SOFTWARE USER MANUAL

UVS Software
for
UVIKON 900 / XL / XS

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1. GENERAL INFORMATION

The user should be, before using the instrument, have read and understood this operating manual, particularly the general warnings given below.

1.1. GENERAL WARNINGS

- *Always disconnect the mains plug before starting any work inside the instrument*
- *Any maintenance operation inside the instrument, including lamp replacement, must be carried out by a service engineer or an authorized person. The user is normally only permitted access to the inside of the sample compartment.*
- *Keep the sample compartment clean*
- *Set wavelength to zero during transport to protect the drive mechanism*

1.2. CD CONTENT

The CD ROM supplied includes :

UVS Spectroscopy Software	Installation program
UVS User Manual	Software User Manual in pdf format
Adobe Acrobat Reader	Installation programs
UVS Software	Validation Certificate

1.3. INSTALLATION and REGISTRATION

The installation and registration procedures are described in a separate document. For the sake of completeness the login and setup procedures are also described in this document.

2. OPERATING INSTRUCTIONS

2.1. INTRODUCTION

This section of the manual describes the various operating possibilities available using the UVIKON. Please note that in all cases it is necessary to follow the general guidelines laid down in section 2.3 dealing with general operation. Examples give a step-by-step introduction to all system methods and calculation modes.

2.1.1. System Icons

The UVS software allows direct selection of many functions via a direct click on the corresponding icon. Many of these icons have the same function in different methods:

Saves the acquired data in the database. In addition, a report-file will be created in the corresponding directory for a given method. These report files can be viewed using the qrv.exe viewer.

Print preview and printing of a report.

Selection mask. You can select a view with date, method, user or name. The appropriate checkbox must be checked.

Transfers data to Excel. Data will be transferred directly to Excel. Excel must be installed for this function to be used. Note that this is not a file export and the data can then only be saved and processed within Excel.

Imports an earlier (extracted) database.

Opens an edit dialogue for reporting functions.

Exports a curve or table to the Windows clipboard for further processing.

Opens the calculation dialogue window or executes a re-calculation.

Opens the audit trail dialogue to allow viewing of the audit trail for a document

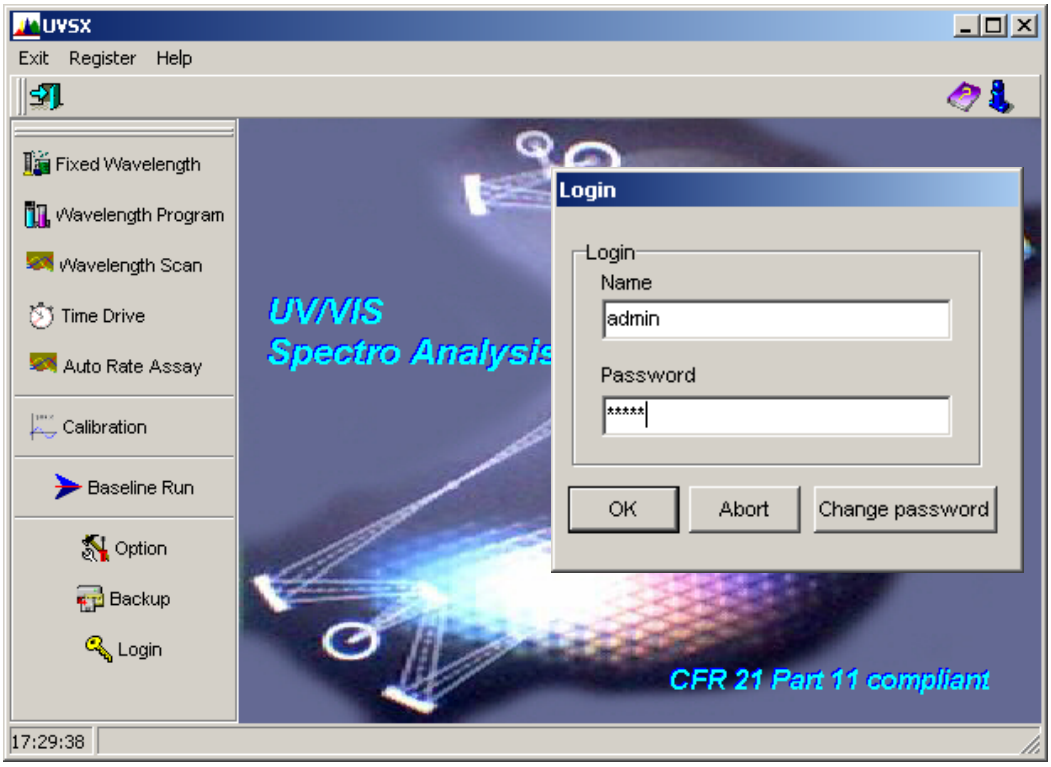
Opens the signature dialogue to allow signing of a document

Shows position of values on X- and Y-axis and allows to manually pick peaks and to add, edit or delete comments.

2.2. SET-UP

2.2.1. Starting

Ensure that the Uvikon is connected to the computer and is switched on. Then click on the UVS icon to start the software. The unit will first initialise, a prompt will appear for user name and password. User name and password are necessary because of the requirements of CFR Part 11 and permit only certain actions for users depending on the assigned permissions.

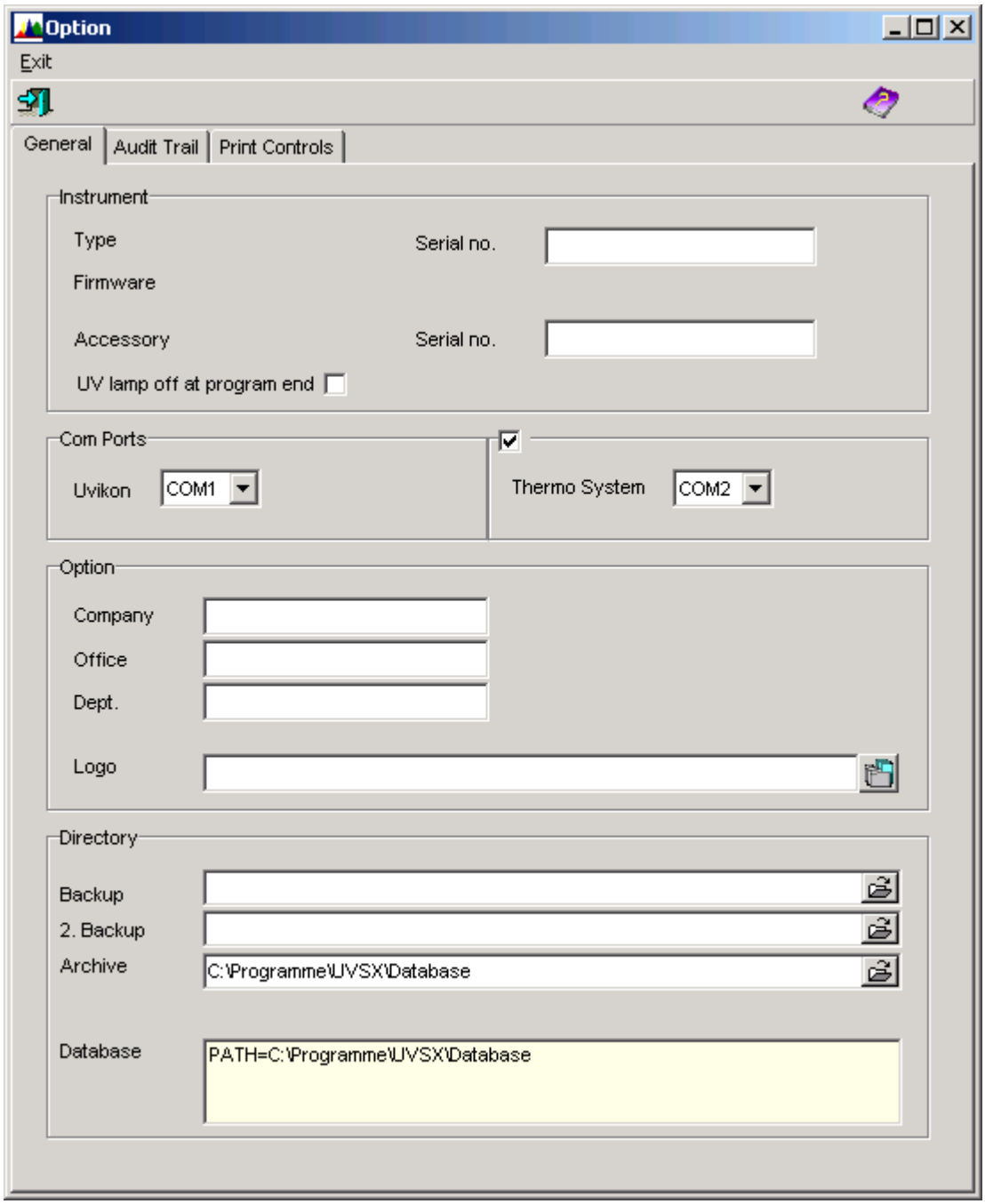


2.2.2. Options

Clicking on *Options* in the main display opens a dialogue window for entry of various parameters relating to reporting and archiving functions of the software.

2.2.2.1. General options

The first window is the “General” window for definition of company name etc. for inclusion on reports and also for the directory locations for the backup and database functions.



Instrument

The section contains data regarding the type of instrument, serial number and firmware used. In addition the accessories are listed and it is possible to enter also manually the serial number of the accessory.

Com Ports

Define the com ports for uvikon (only UVSX) and thermo system if needed, disable thermo system checkbox if no thermo system is connected.

After changing com ports please start UVS again.

Options

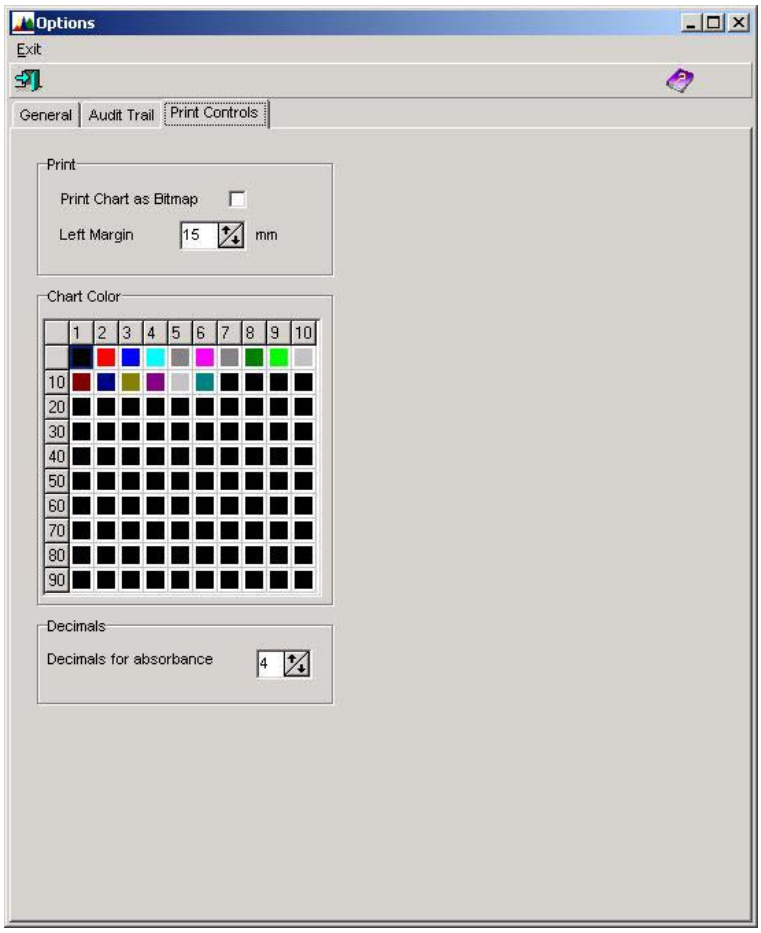
These options define parameters which are included in the standard reports. Under Logo the location of a company logo file can be defined which is included in every printed report.

Directory

Here the location paths for the backup directories and database are defined. Definition of a second backup location is not necessary but recommended.

2.2.2.2. Control options

The second window is accessed by clicking on the “Controls” tab and allows control of chart print format, chart colour, decimal points for diplayed absorbance values and audit trail.



Audit Trail Functions

Error messages An audit trail for all error messages will be kept if this function is checked.

Report revision If checked and changes are made to a report then a copy of the original will be made and the revision number incremented. If this function is not checked, any change will automatically overwrite the earlier version.

Method revision If “**All methods**” is checked and any changes are made to a method, a copy of the original will be made and the revision number incremented.

If “**Only with used methods**” is checked, changes and modifications to a method will not be tracked under revision control until the method has been used for data acquisition and the corresponding report has been saved. This is the recommended setting.

If "**None**" is checked, any change will automatically overwrite the earlier version.

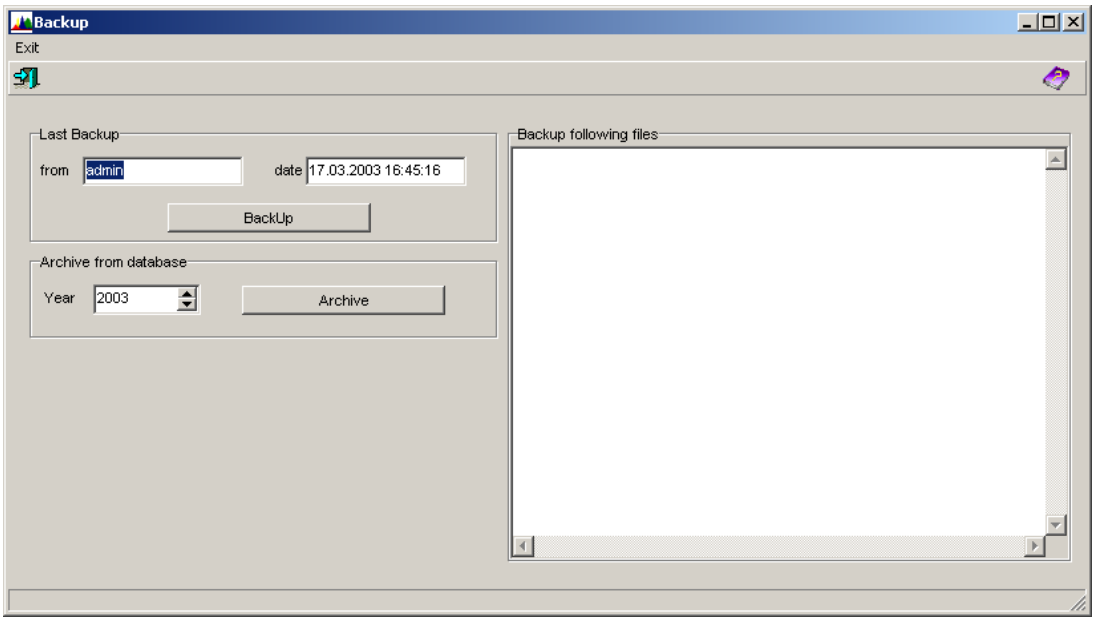
Report trail An audit trail for all changes to reports will be kept, if this function is checked.

Chart colour Colour table for curve colours in the order in which the curves are acquired. The colours may be selected individually.

2.2.3. Backup

This function permits a backup or archive of either all data or an extract from the original database to a database sorted by year is possible.

The backup can be made to 2 independent servers via network, if the appropriate directory locations have been entered in the options section.



2.2.3.1. Backup

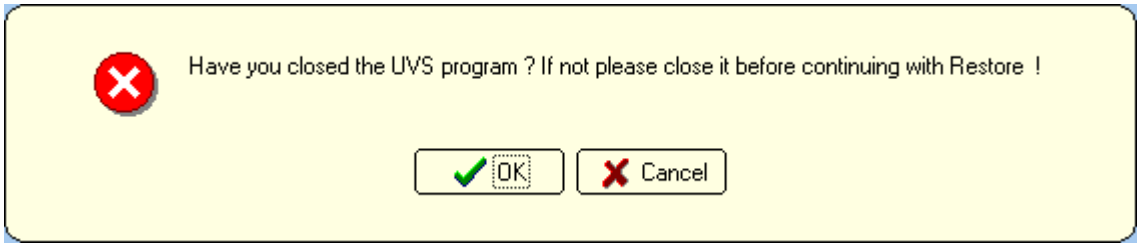
Clicking on the *Backup* button will execute a backup of the complete database to the directory locations defined in the Options menu. The right hand panel will display a listing of all files which will be backed up during the process. A confirmation dialogue is shown after successful execution of the backup:

The backup simply saves a copy of the working database files to the defined locations from which they can also be restored at any time as described below.

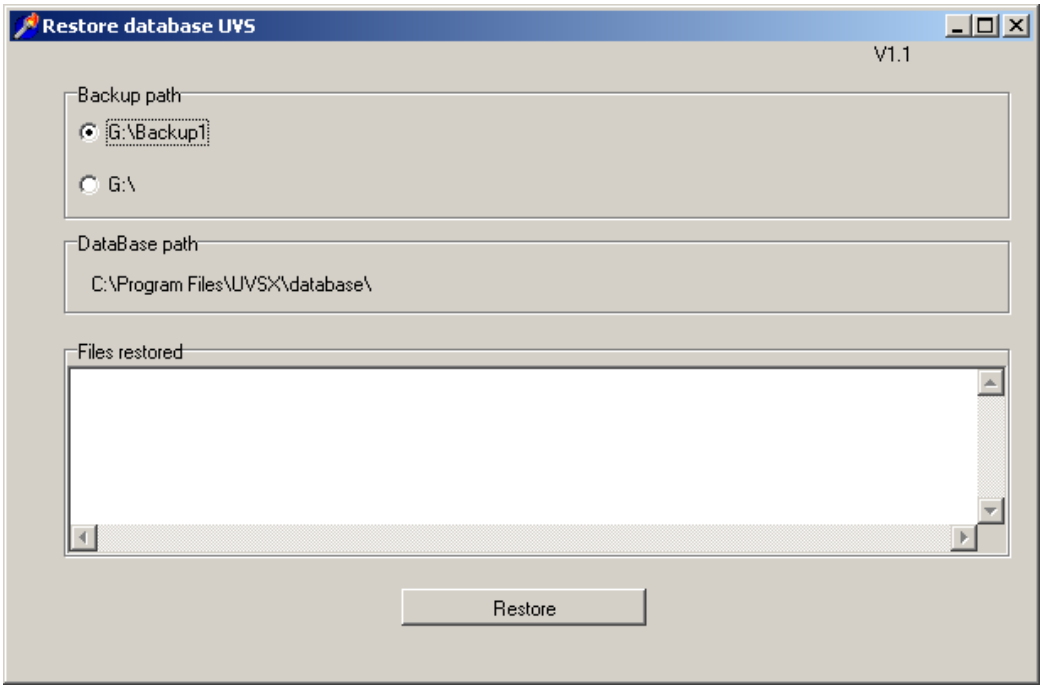
2.2.3.2. Restoring Backup Data

Restoring of previously backed up data is possible using the “restore UVS” application located in the UVS directory. In order to restore data you must close the normal UVS software before starting the restore process, a prompt will remind you of this before continuing:

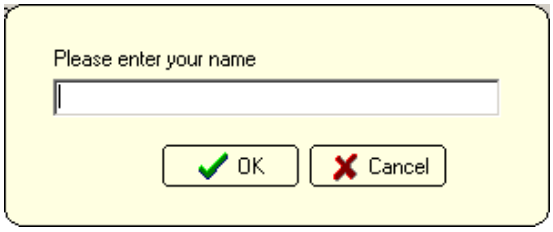
Start the restore UVS program, a prompt will appear to check that the main program has been closed:



Close if necessary and click on *OK* to obtain the restore dialogue:

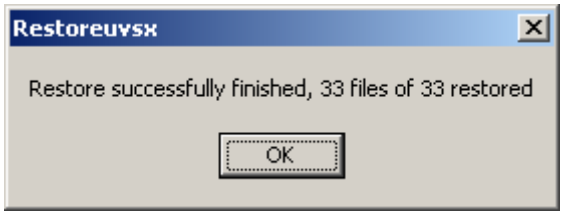


Specify the location from which you want to restore the data and click on the *Restore* button. You will be prompted to enter your name:



This name is required for record purposes and does not correspond with the user names installed for the main UVS software. Enter a name and click on *OK*.

The restore process will be confirmed:



2.2.3.3. Archive

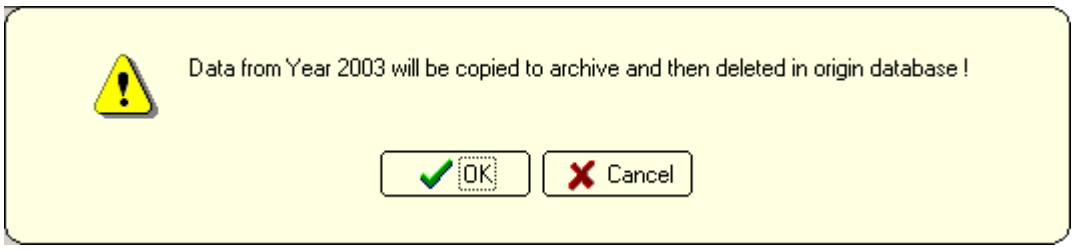
The archive is based on data obtained within any given year, e.g. all data collected during 2003. The data is then archived in the database and the original data removed locally.

Caution *It is possible to restore Archive data for viewing and modification during a working session. However, the restored data is automatically removed locally whenever Exit is executed. Modifications made during a session are automatically added to the archive data when exiting.*

The archive is not intended for storage of data which will be needed for comparison etc. Therefore, great care must be taken to select the ideal time to archive all data.

It is also possible to selectively control archiving by using the file based backup program module to save data before deleting that data in UVS which does not need to be archived immediately. The original data can then be restored as described above and the archived data removed.

The location of the archived database is pre-defined in the options page in the UVS software and therefore the user need only define the actual year to be archived and then click on the *Archive* button. A prompt appears requesting confirmation:



Click on *OK* to complete the archiving process.

1. Menu item: Options

↳General Options

Setting the directories for Backup and Archive

Archive

Execution of Archiving in the Backup window of the main menu.

Prior to execution the year can be selected.

Backup

Execution of Backup in the Backup

Is saved with the Backup if a directory for the Archive was selected in the **`Database`** directory

Re-importing data from an Archive

Selection is made in the Report menu of a Method

- Selection of the year lists the corresponding data for the selected year
- Data can be re-calculated and partially combined (only within a given year)
- In the Report a range of search filters is available (Date, Text, etc.)
- The copying of data from one archive into another archive or the current data base is not possible.
- Users and Powerusers can also call up and re-process archived data, if the appropriate permissions in User Management have been set.

All files are saved in the **`Database`** directory.

(including sub-directories)

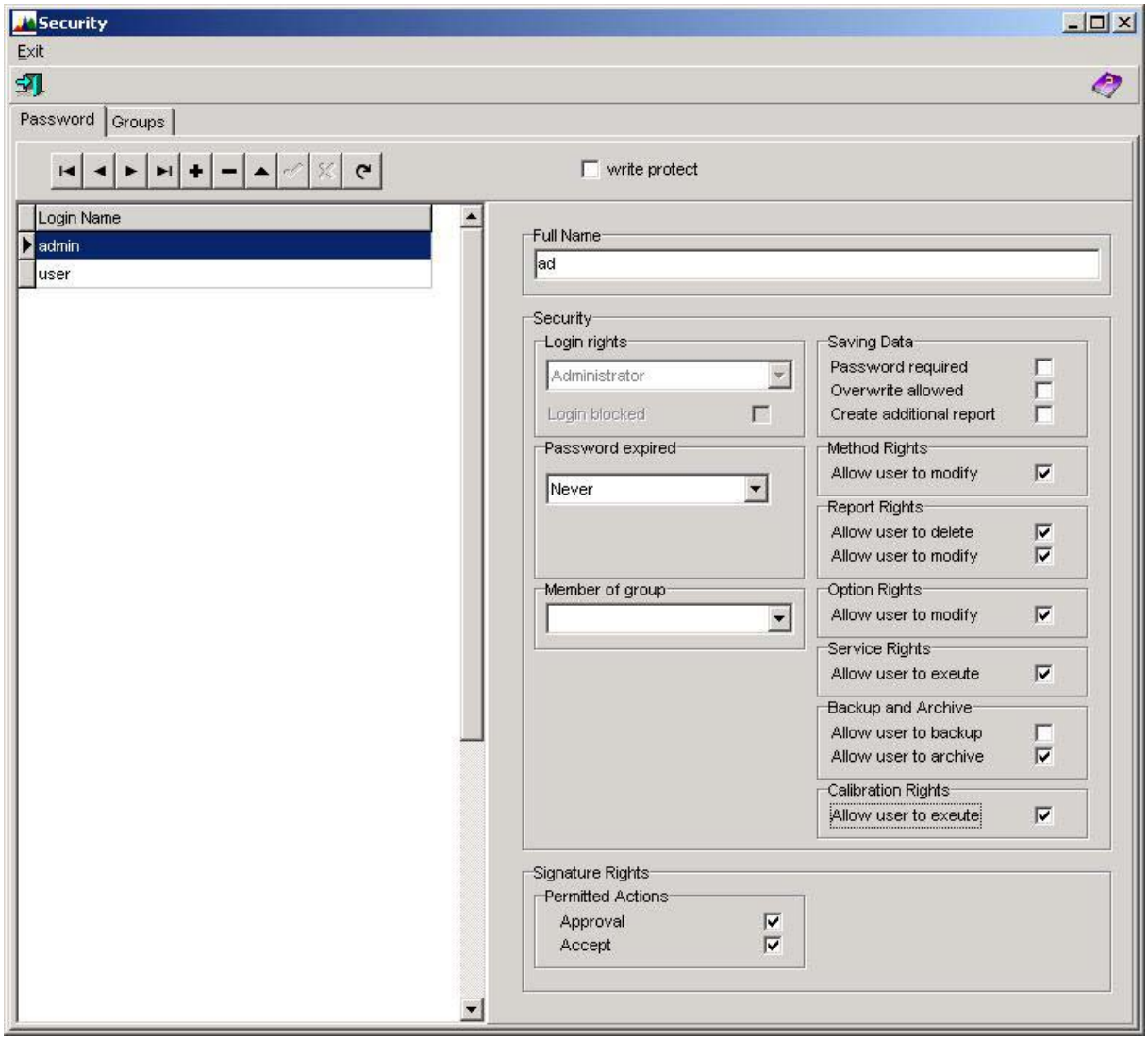
Two files are created:

`*.bck` File extension for the re-importing using the „Restore“ tool supplied

`*.zip` File extension for the manual re-import procedure using an „Unzip“ program, e.g. Winzip

2.2.4. User management

has its own login facility. A login name and a password is required to enter the program. The assignment of user rights, password administration etc is made by the administrator in a separate dialogue box accessed by clicking on the *Login* key in the main display.



2.2.4.1. **Password**

2.2.4.1.1. User rights

Generally three different user types are recognised with basic default permissions as described below:

	Action	Administrator	Power User	User
Main window	Fix Wavelength	yes	yes	yes
	Wavelength Program	yes	yes	yes
	Scan	yes	yes	yes
	Timedrive	yes	yes	yes
	Autorate Assay	yes	yes	yes
	Calibration	yes	Depends on security rights	
	Baseline Run	yes	yes	yes
	Option	Depends on security rights	Depends on security rights. Access only to print controls	Depends on security rights. Access only to print controls
	Backup	yes	Depends on security rights	
	Edit Security	yes	no	no
	Trail	yes	yes	yes
	Service	Depends on security rights		
Checked security rights	Password required on saving data	Depends on security rights		
	Overwrite existing report on saving data	Depends on security rights		
	Create additional report on saving data	Depends on security rights		
	Change Method	Depends on security rights		
	Delete Report	Depends on security rights		
	Modify Report	Depends on security rights		
	Signature approval	Depends on security rights		
	Signature accept	Depends on security rights		
Visibility	Report	all	Only own or grouped member reports	Only own or grouped member reports
	Method	all	all	all

The permissions for individual users are modified by the administrator by checking the appropriate boxes.

2.2.4.1.2. Adding users

In order to add a user it is always necessary to unclick the “write protect” checkbox and the click on the “+” or “-“ symbols to add or remove a user respectively.

Click on “+” and a dialogue box will prompt for a new user name:

Enter a name and click on *OK*, the new user will be entered in the list and the permissions for the new user can be selected using the dialogue boxes on the right of the window:

2.2.4.1.3. Login rights

Clicking on the drop-down arrow cause the three possible user types to be displayed as a drop-down list. Select the required user type from the list.

2.2.4.1.4. Login blocked

Clicking on this checkbox can be used to prevent a user from accessing the system temporarily. Permanent exclusion of a user should be made by deleting the user completely from the list using the “-“ button.

2.2.4.1.5. Additional Rights

Users can be assigned the right to delete reports. If this checkbox is not ticked the user is not allowed to delete reports.

2.2.4.1.6. Saving data

Clicking on the “Password required” checkbox will activate a password dialogue in order to permit saving of the acquired data. This security feature can be used to identify those users allowed to save data. Only the currently logged-in user provided with the appropriate rights can save data.

Clicking on the “Overwrite allowed” checkbox allows the user to also overwrite previously saved data.

Clicking on the “Create additional report” checkbox allows the user to save additional reports after creation of the initial report using the same acquired data.

2.2.4.1.7. Password expired

A change of password can be forced at certain intervals as defined by this dialogue. The option of never changing is also available but users should note that this option is not acceptable when operating in a controlled environment.

Entry of a time interval automatically produces a new box with the actual date by which the password must be changed.

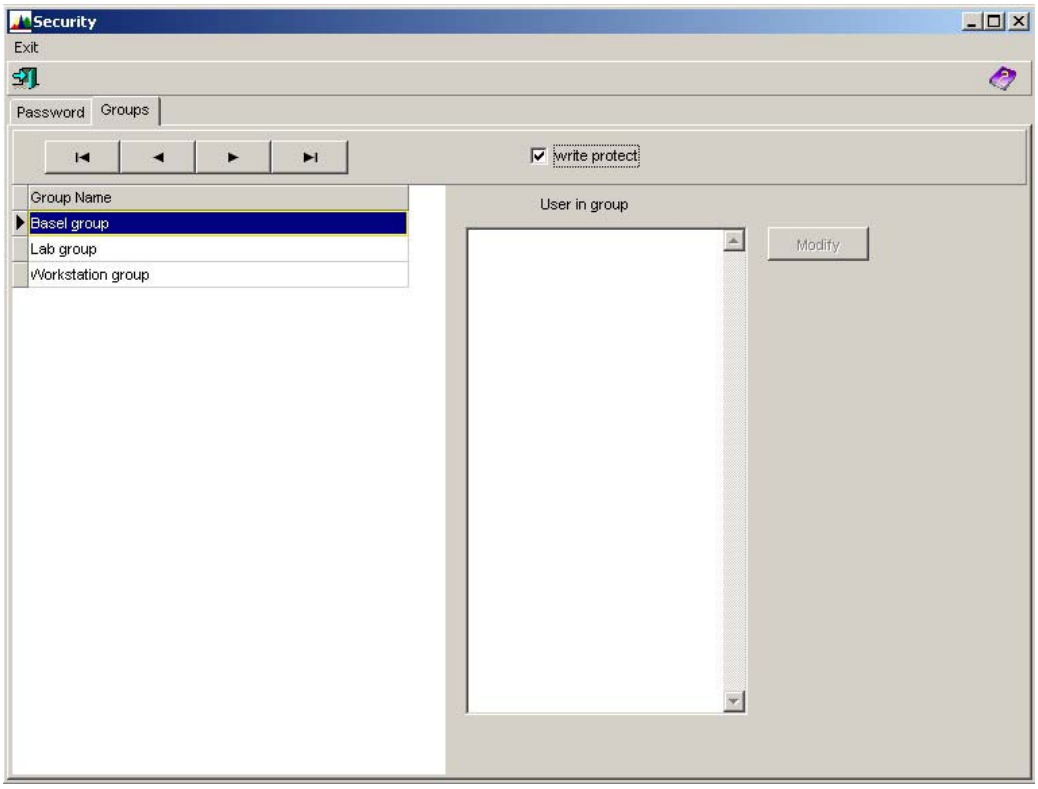
2.2.4.1.8. Password

This allows definition of the user password for normal access control and also for saving of data if the checkbox described is activated.

The initial password for the new user must be entered in the appropriate box. New users will be forced to change this password when they log onto the system for the first time. This is a precautionary measure to ensure that the system access password is known only to the user and no other third-party.

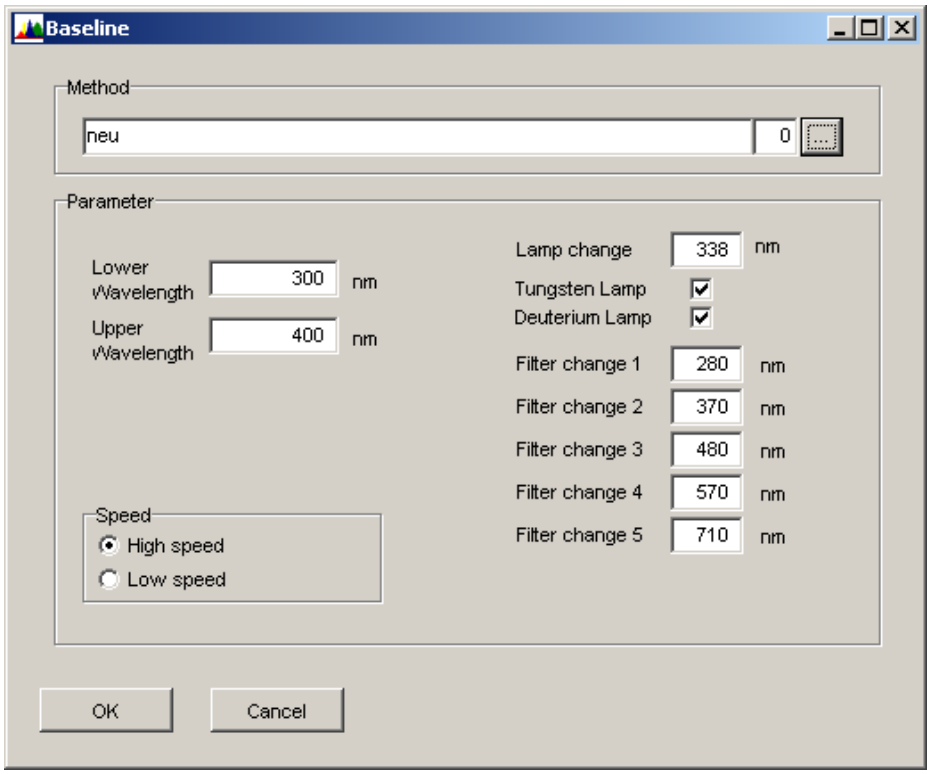
2.2.4.2. Groups

This defines the grouping for report access. Groups and members of groups can be defined to view the reports. A member of a group can view the reports of all members.



2.2.5. Baseline

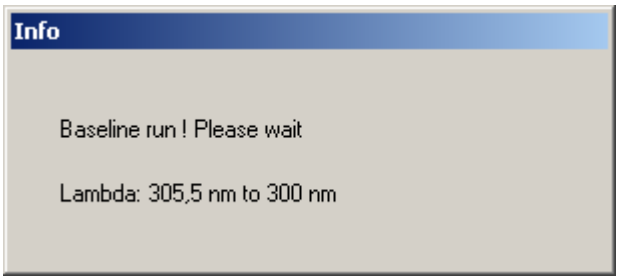
The UVS software does not automatically execute a baseline at start-up. This operation can be executed by clicking on the *Baseline Run* icon in the start-up screen to open the following dialogue window:



The actual conditions under which a baseline is executed can impact later measurement results if these are made using different parameters such as scan speed. For this reason the UVS software requires a method to be defined in *Wavelength Scan* mode before a baseline can be executed.

Click on the selection button adjacent to the method box in order to select the correct method if this is not already displayed. This method is then displayed before starting a baseline but can only be edited in the method editor itself thus permitting tracking of baseline conditions during normal operation.

Click on *OK* in order to start the baseline measurement, the unit will position itself at the correct starting wavelength and then automatically start the run:



2.2.6. Power on

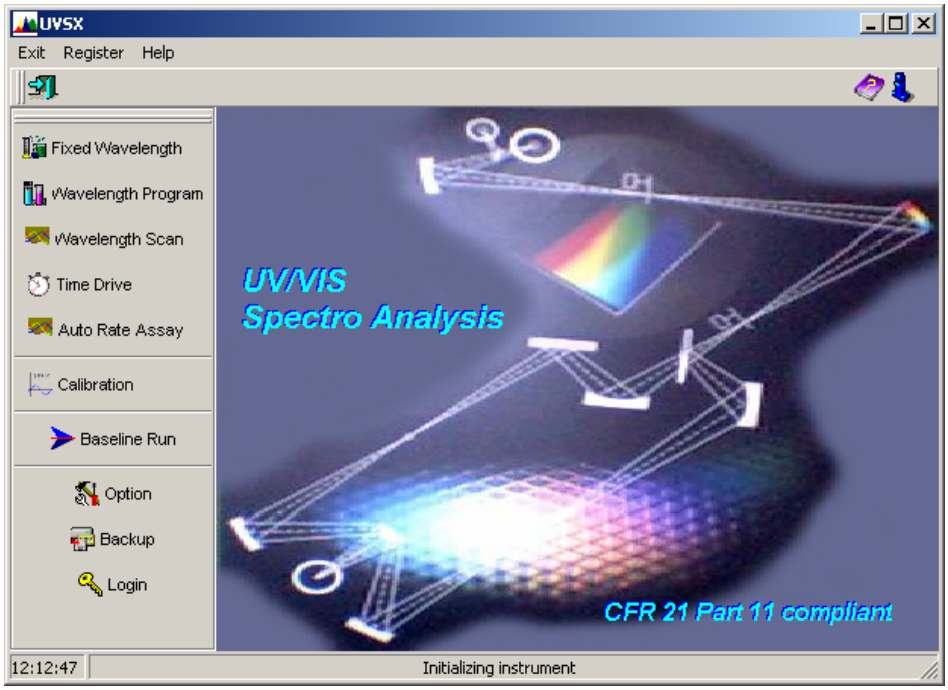
Switch on the power supply to the instrument, PC and monitor. The Uvikon has an indicator showing that the power is on. From the Windows Desktop click on the shortcut to display the start-up screen and login dialogue.

2.2.7. Self test and system software initialisation

The self test takes about 2 minutes (max) and performs the following checks:

- Program memory
- Data memory
- Tungsten halogen lamp on
- Deuterium lamp on
- Data transfer
- Wavelength drive

During self test you will see the main software window on the screen with "**Initializing instrument**" displayed on the bottom status bar.:



After completion of the initialisation this message will disappear and the software will prompt for user name and password for log in.

2.2.8. Exiting the system software

You can exit the system software by clicking either on the *Exit* icon in the top left corner or on the "**X**" in the top right corner.

2.3. OPERATION

2.3.1. General guidelines

2.3.1.1. Acquisition-Calculate-Display

The UVIKON uses an **A**cquisition-**C**alculate-**D**isplay scheme as shown below:

Acquire data for 1 to 10 samples using method parameters	➔	**C**alculate 1 to 10 samples using method parameters	➔	**D**isplay results of 1 to 10 samples using method parameters

The system is structured to use individual measurement modes, e.g. *Fixed Wavelength*, which must be pre-selected by the user. The selection of the mode to be used is made in the opening screen which can be accessed immediately after the software has started and login has been completed. This screen can also be reached at any time by exiting from the current mode in use.

2.3.1.2. Recommended Operating Practise

Each measuring mode uses *Acquisition* parameters which must be pre-defined in a *Method*. The *Method* also contains the data necessary for the final display of the results in the form of a *Report*.

The *Method* is the key to maintain a trace to all results and, together with the different reports, is subject to a strict revision control including an audit trail.

The method to be used can be selected from within the *Acquisition* page, where also the naming and number of samples to be analysed can be defined.

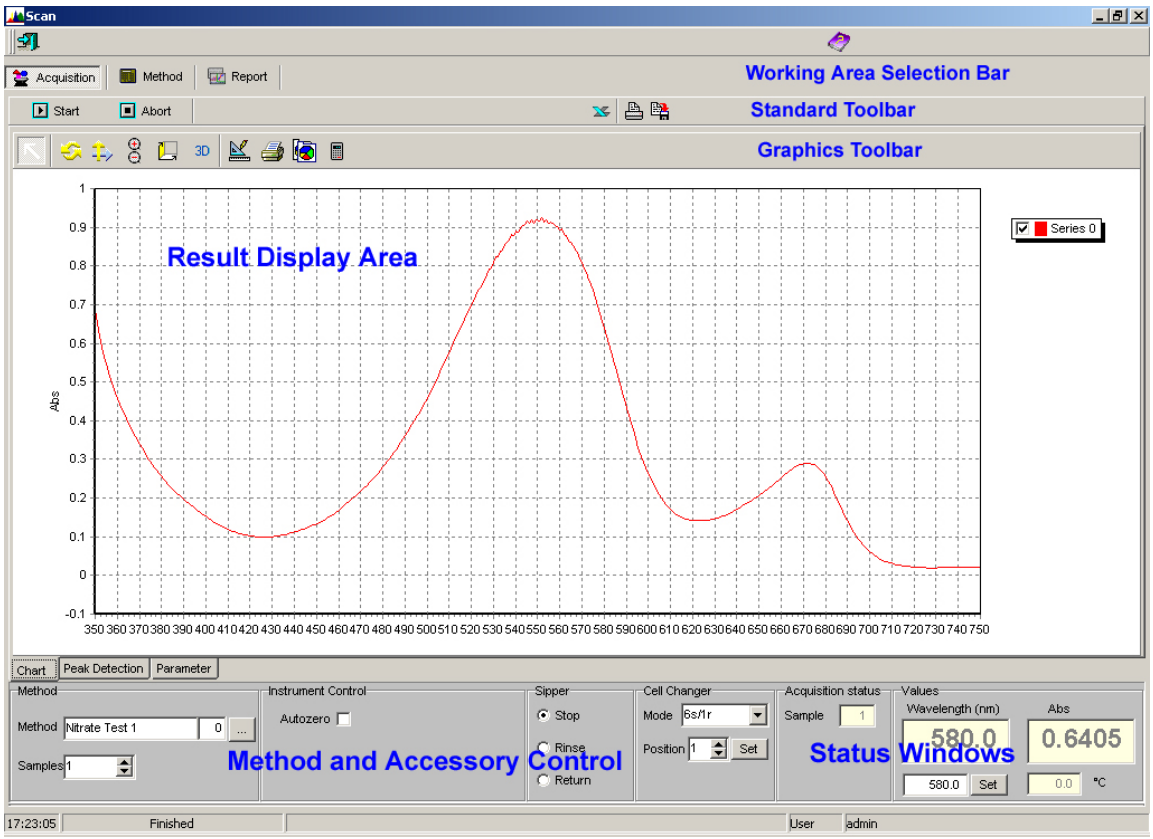
For routine testing the various *Methods* to be used will normally have been pre-defined and therefore it should not be necessary for users to access the *Method* screen. All necessary entries for simple routine operation with a series of samples can therefore be made directly in the *Acquisition* area.

A result report can also be previewed and printed directly from the *Acquisition* area and is therefore not necessary for the user to switch between the various main windows.

The individual windows for the three main operating areas are accessible via main buttons in the top section of each window and are described below:

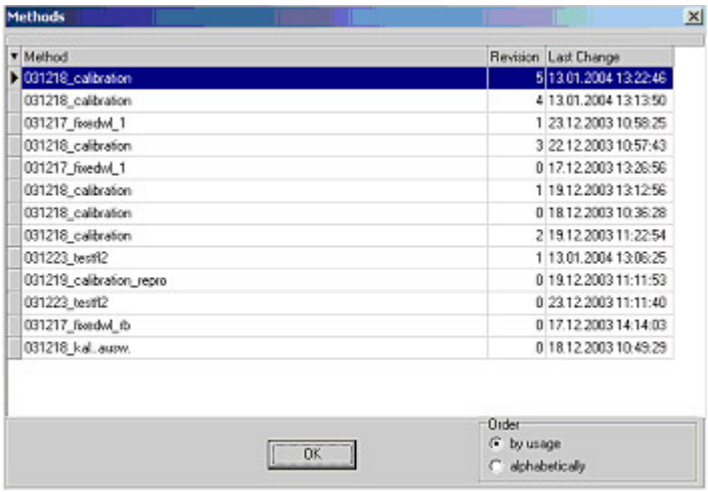
2.3.1.3. The Acquisition Window

The *Acquisition* page layout is similar for each mode and is shown below. A graphical display is only available for those measuring modes where graphics are actually required and used, e.g. *Wavelength Scanning*.

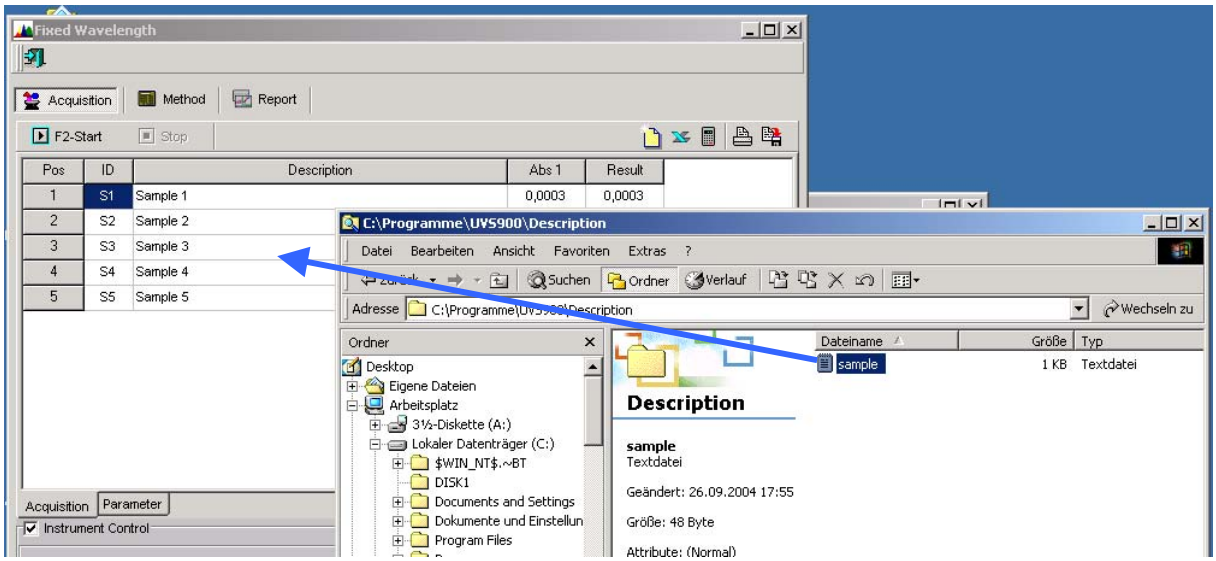


Working Area Selection	Buttons for selection of working window, e.g. *Method*.
Standard Toolbar	Contains buttons for starting and stopping measurements plus Excel export, printing and saving data for the currently open document.
Graphics Toolbar	Contains all functions required for controlling the appearance of the curve display, these are described in more detail below.
Status Windows	The status windows shows the current or last instrument status.
Method & Accessory Control	Enter the method name and the number of samples to be analysed.

The list for selecting methods may be sorted alphabetically or by the access counts. The most used method is on the top.

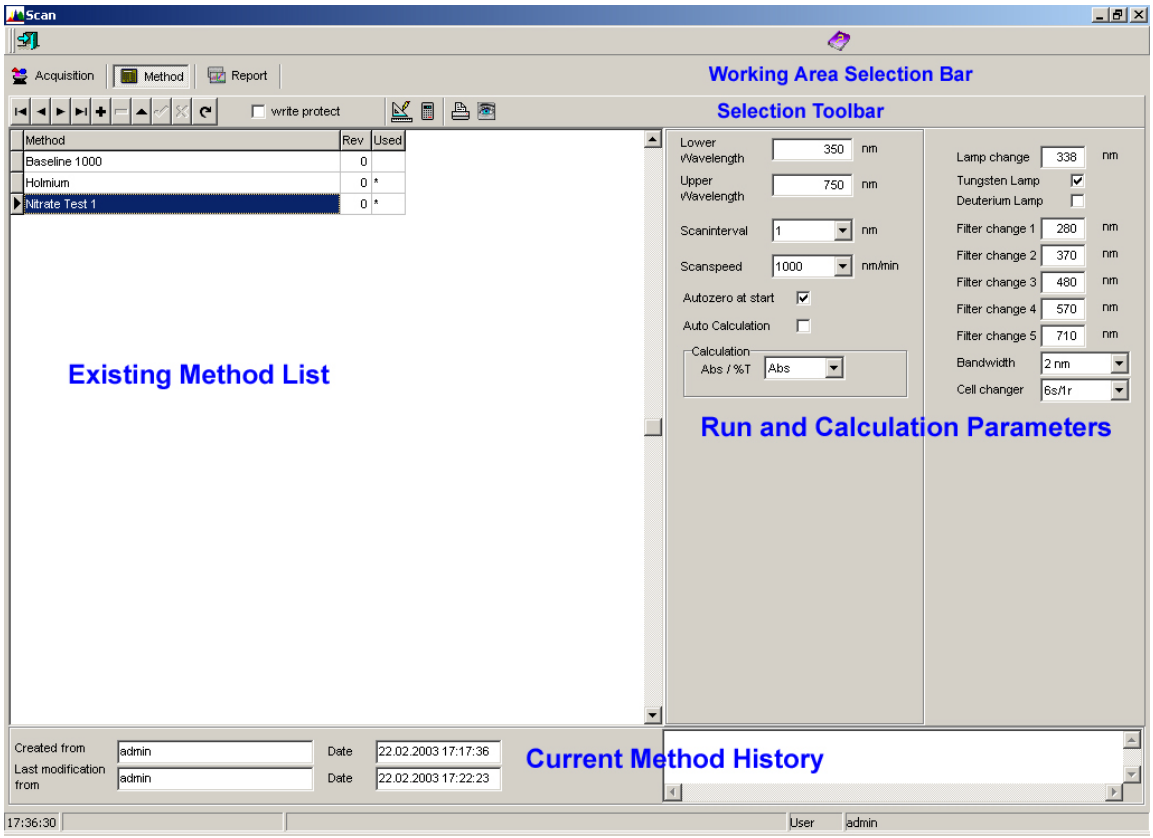


The sample description can be imported from a text file from the explorer via drag and drop.
Select the text file in the explorer and drag it with left mouse button pressed to the description grid.
Then release the mouse button, the text is dropped into the grid.



2.3.1.4. The Method Window

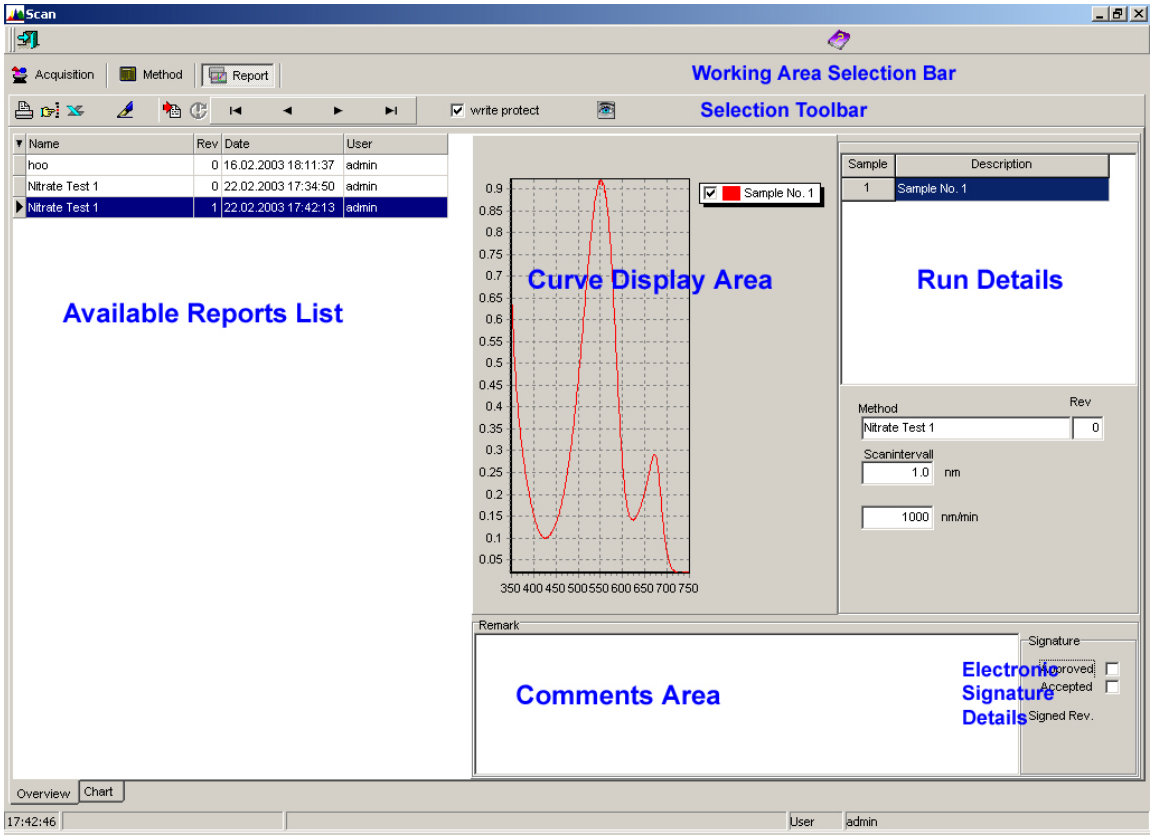
The *Method* page layout is similar for each mode and is shown below. Graphical display functions are again only available in those measuring modes where graphics are actually used, e.g. *Wavelength Scanning*. Other functions such as calibration definition are also not present in every window.



Working Area Selection	Buttons for selection of working window, e.g. *Method*.
Selection Toolbar	Contains buttons for navigating the current method list plus buttons to allow addition or deletion of methods.
Existing Method List	Contains a list of all methods used for the given measuring mode. Scrolling through the list updates automatically the corresponding fields in the parameter definition fields.
Parameter Definition	All parameters necessary for the method are defined and displayed here.
Current Method History	Displays data relevant to the creation and history of each method in the list.

2.3.1.5. The Report Window

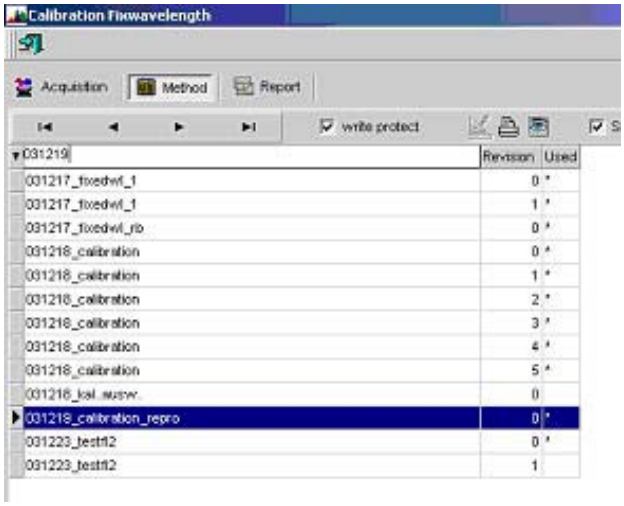
The *Report* page layout is similar for each mode and is shown below. Graphical display functions are again only available in those measuring modes where graphics are actually used.



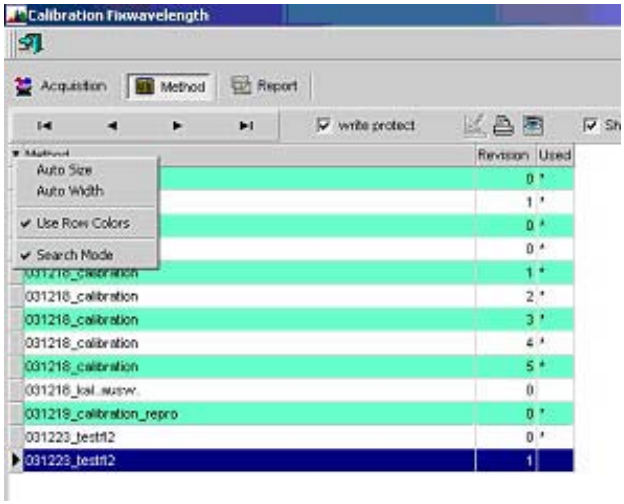
Working Area Selection	Buttons for selection of working window, e.g. *Method*.
Selection Toolbar	Contains buttons for navigating the current list plus buttons to allow archiving or printing of reports.
Available Reports List	Contains a list of all reports available used for the given measuring mode. Scrolling through the list updates automatically the corresponding fields in the results area fields.
Curve Display Area	Shows all curves available for the current report.
Comments Area	Displays data for the samples contained in the current report.
Electronic Signature	Shows details relating to status of electronic signature for a report.

2.3.1.6. Quick Search Function and Row Colouring

In Methods and Reports a quick search function may be used to quickly find the required file. Therefore, click on the fixed row to enter the name of the file. It will be highlighted automatically.



Also, by clicking on the small arrow in the left corner of the fixed row, the rows may be coloured.



2.3.2. Starting a measurement

The **"Start"** button on the main menu bar is used in all methods to start measurement of one to ten samples. All parameters defined in the selected method are then used for a measurement.

Measurement can be stopped at any time by pressing the **"Stop"** button on the main menu bar. All data measured up to that point is valid and can be stored and used for further processing.

2.3.3. Recalculation

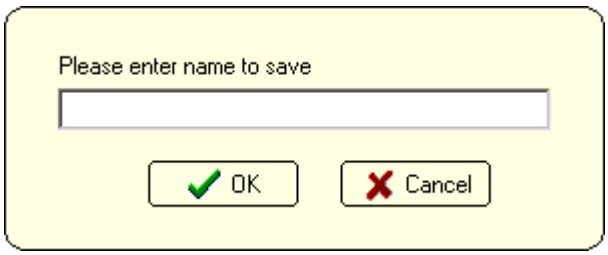
The calculations are made automatically as part of the acquisition process in the UVS software. In cases where parameters are changed a recalculation can be forced as described below.

Clicking on the *Calculator* icon on the tool bar is used throughout the software package to initiate a re-calculation of one to ten samples. Only the parameters in the calculate column and the display column of the acquisition parameter set are used for calculation.

2.3.4. Saving data

Clicking on the "**Save**" button on the toolbar allows the currently displayed data to be saved. The following dialogue box appears:

Enter the required file name in the input window and click on the *OK* button.



2.3.5. Loading existing data files

Data which has already been acquired can be viewed via the main *Report* window in any of the measuring modes.

Select the *Report* window by clicking on the *Report* button. The left hand section of the window contains a list of acquired data files which can be viewed and loaded by clicking on the appropriate line.

2.3.6. Data conversion to EXCEL format

Data files can be converted directly to Excel® (*.XLS) format to be read from Excel spreadsheet programs. Excel must be installed for this function to be used. The data will be transferred directly to Excel and can then only be saved and processed within Excel.

Caution: *This data cannot be re-imported into the UVS software and is not subject to any further controls by the UVS software with respect to security considerations for electronic documentation.*

Click on the icon to transfer data to Excel. Excel is opened automatically and the data entered in a worksheet.

2.3.7. Export to Clipboard

Data files in graph format can be exported to the *Windows Clipboard* to be immediately imported into other running programs via the copy-paste mechanism.

Click on the clipboard icon in the graphics toolbar and the curve is exported automatically to the clipboard for further processing.

2.3.8. Methods

The system will always use a set of parameters called a "*Method*" to execute the data acquisition and measurement step.

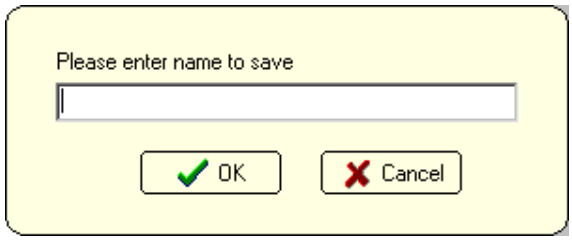
The method file for an acquisition is selected from a drop-down list in the main acquisition window as described below each measuring mode. Simply click on the required method in the list.

Programming and viewing of methods is made from the *Method* screen for each measuring mode. Existing methods are shown in a list in the left-hand window, clicking or scrolling through the list allows an easy overview of the current method in this list.

A new method is programmed by removing the "write-protect" check box tick and clicking on the " + " icon. The available functions for each method type are described in the appropriate sections below.

2.3.9. Saving methods

The system prompts for a name for the method to be stored whenever a new method is to be created. Generally methods cannot be simply overwritten because of the tracking system used for CFR Part 11 therefore it is necessary to enter a new name and confirm with *OK*.



Once the parameters for the method have been entered the method is saved by clicking on the green tick in the option tool bar:

2.3.10. Cancel all current activities

Clicking on the *Exit* icon in the top left-hand corner of each screen will return automatically to the start-up screen.

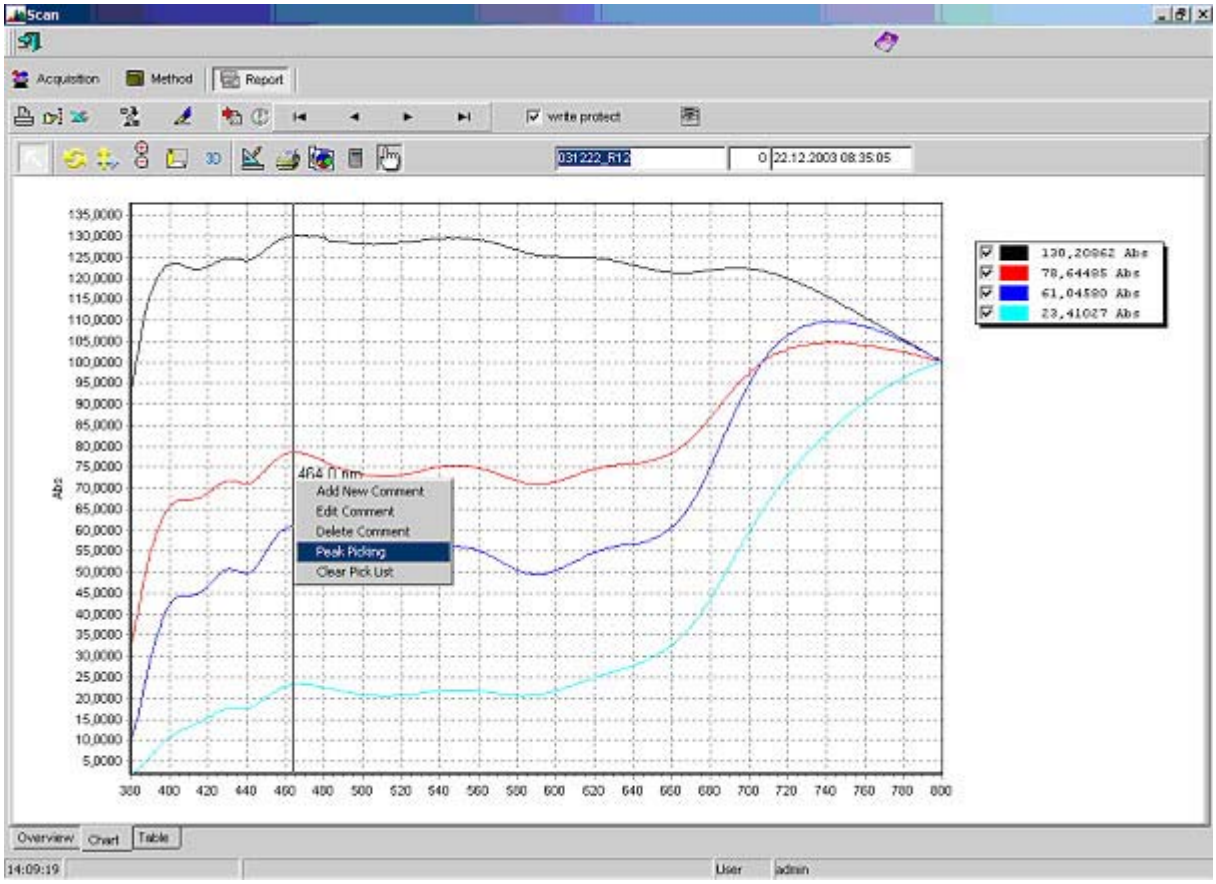
Clicking on the “Stop” button in the acquisition screen will cancel any currently running data acquisition etc.

Caution *If you exit without having saved your data on disk you cannot restore the data. A message will warn you if this situation occurs.*

2.3.11. Activate Cursor and Manual Peak Picking

The *Activate Cursor* icon can be used in *Wavelength Scan*, *Time Drive* and *Auto Rate Assay* methods to quickly overview values of the sample curve on the screen.

In the *Report Overview* window click on the chart tab to obtain the curve display. Click on the *Activate Cursor* icon. A vertical cursor can now be moved across the curve graph and the values for the wavelength are continuously displayed on the cursor line. The arrow used to move the cursor is also used for the position of the Y-axis and values for the current Y-position are continuously updated in the legend window adjacent to the curve.
Additionally, by clicking on the right mouse button, you may add new comments, edit and delete comments.



When the cursor is activated, you may manually pick peaks by clicking the right mouse button and choose *Peak Picking*.
You can also activate or deactivate samples in the legend.

2.3.12. Zooming

Zooming is available for all methods where graphical curve displays, e.g. *Wavelength Scan*, *Time Drive* or *Auto Rate Assay*, are available and is used to magnify a section of the graph.

Simply move the cursor on the graph to the upper left corner of the rectangle to be magnified, press the left button of the mouse and move it to the right while keeping the left button pressed. A rectangle will be shown on the screen indicating the area that will be magnified.

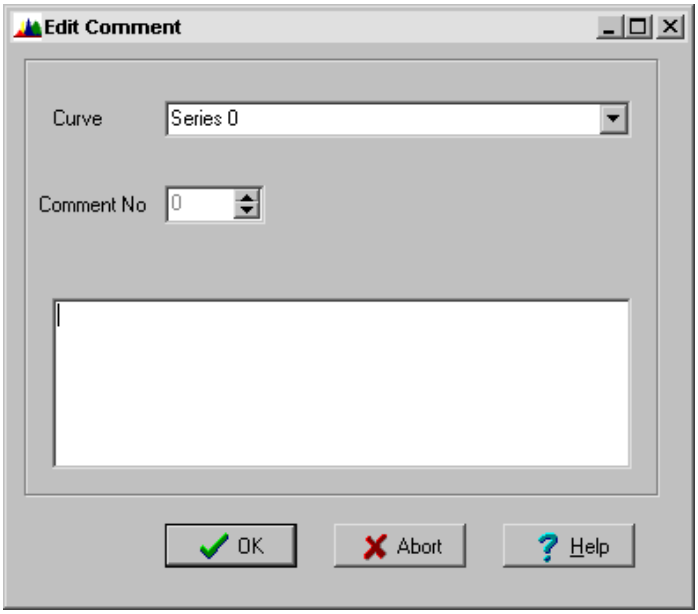
When you reach the lower right corner of your area, release the button and the area selected is zoomed to fill the graph area.

You can repeat the zooming function up to the maximum resolution by repeating the selection of the zoomed area.

To unzoom simply position the cursor on the graph, press the left mouse key, move the cursor to the left and release the left mouse key or double click with left mouse key.

2.3.13. Adding comments to curves

You can add a comment at any point on a curve for documentation purposes. When a curve is displayed on the screen, click the *Activate Cursor* icon in the Graphics toolbar, move the mouse cursor to the point on the curve where the comment should be added and click the right mouse button. A small dialogue box appears offering the choice of adding, editing or deleting a comment. Click on a selection and the appropriate dialogue window will appear:



Input the desired comment text using alphanumeric characters and press "**OK**". The comment will appear directly linked to the curve at the cursor position on the X-axis.

More comments may be added by repeating the same procedure. The comments are numbered and the spin selector by the *Comment No* box can be used when editing or deleting comments in order to select the item to be used.

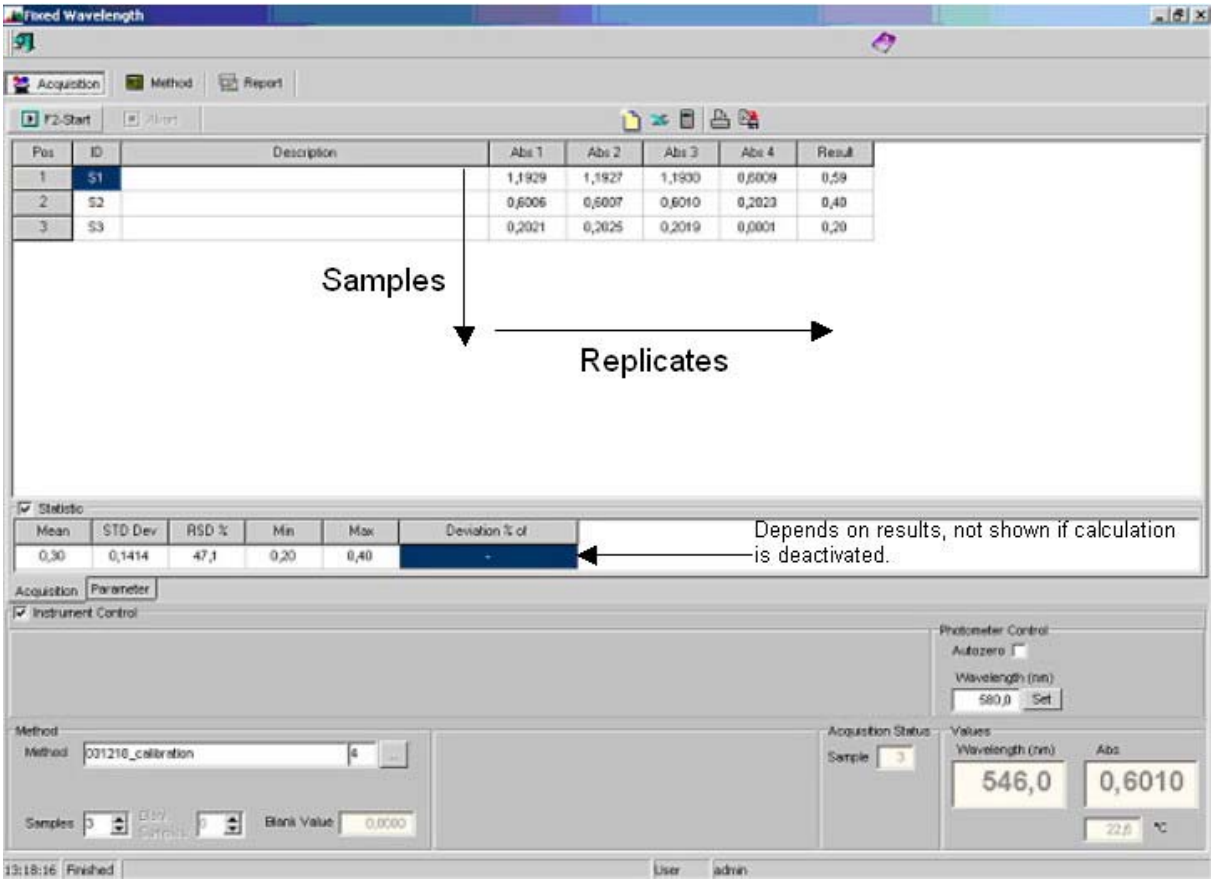
2.4. SYSTEM MODES

This section explains the parameters and gives a step by step measurement example for each system mode. Many parameters are common to all methods but are explained separately for each mode in the interests of clarity.

2.4.1. Fixed Wavelength

2.4.1.1. The Acquisition Screen in Fixed Wavelength

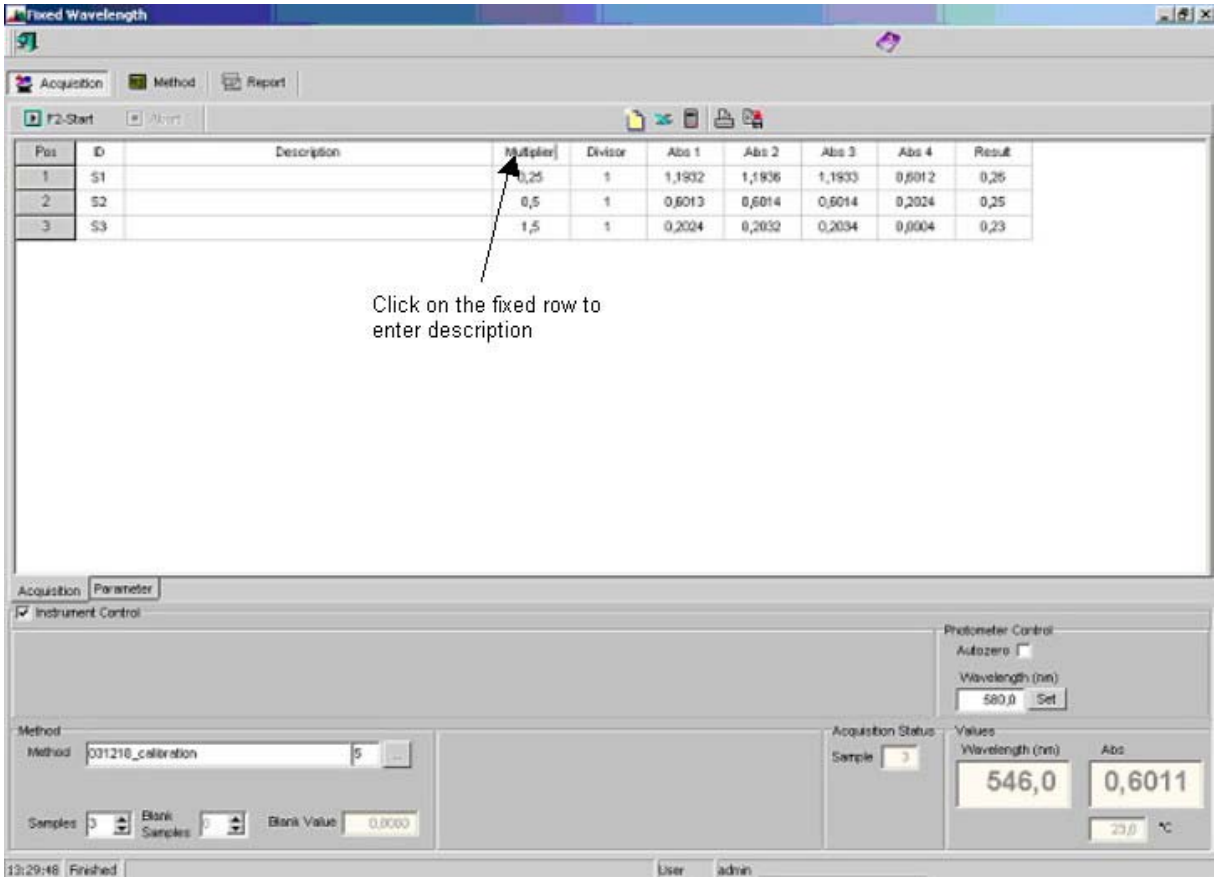
Select **"Fixed Wavelength"** from the main menu to obtain the following display:



This is the acquisition window from which all measurements are started. In this window the following parameters must be selected before starting a measurement:

- Method to be used for the acquisition. The method contains all parameters necessary for the execution of the measurement.
- Numbers of samples to be measured.
- Number of blank samples, measured as the first samples.
- *Autozero* at start of measurement.

If Individual Multiplier / Divisor is activated in the Method, you may add a multiplication / division factor before the measurement values. Both, multiplier and divisor, have to be defined. The factor not used should therefore be set to “1”. E.g. if you choose the multiplier of 1.7 for a sample, you have to set the respective divisor to 1. The calculation will be applied by clicking on the *Calculate* icon in the selection toolbar. You may also define a description for the factor by clicking on the fixed row to enter description.



2.4.1.1.1. Statistic

If *Calculation* is activated in the *Method*, the calculation of mean, standard deviation, RSD %, min., max. and the deviation percentage of the mean regarding sample no. 1 will be shown.

If *Concentration* is activated in the *Method*, a chart is shown with the concentration values and the regression curve.

2.4.1.1.2. Instrument Control

Autozero may be activated before starting a measurement.

2.4.1.1.3. Run parameters

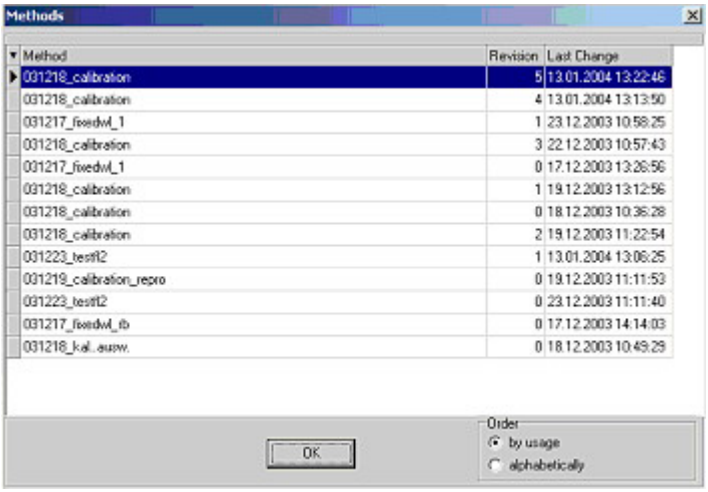
The run parameters are entered in the lower left section of the screen:

Samples Defines the number of samples to be analysed.

Blank Samples Defines the number of blank samples to be measured, blank samples are always expected at the start of a run. The value of the measured blank is subtracted from the actual measured value of the sample prior to calculation of concentration etc. If more than one blank is defined then the system calculates the average blank value for the blanks and then subtracts this from the actual measured sample values.

Method The method box contains the name of the method and, directly adjacent, the actual revision number of that method. The method is selected from a separate window which opened by clicking on the button adjacent to the revision box:

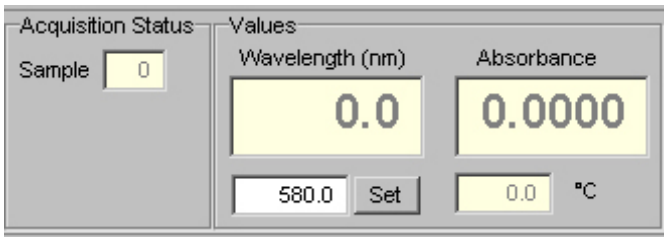
Thermo System Surveys the temperature of the sample



This window contains a list of all available methods including all revisions of the method and the date of last modification. The order of the shown methods may be selected by ticking “by usage” or “alphabetically” in the lower right corner of the screen. Selection is made by highlighting the required line and then clicking on *OK*.

Cell Changer The operating mode of the cell changer and the actual position can be defined here beforestarting a measurement series.

2.4.1.1.4. System Status



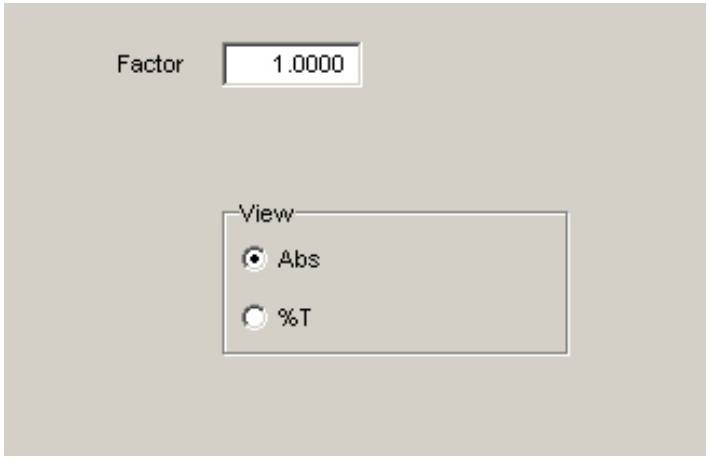
The lower right section of the display contains the actual status of the system and displays the following parameters:

- Current sample being measured.
- Actual wavelength.
- Actual absorbance value.
- Temperature (where applicable).

In addition the lower right panel also allows manual setting of wavelength in order to allow rapid monitoring of the unit.

2.4.1.2. Parameters in Fixed Wavelength Acquisition

Clicking on the parameter tab in the acquisition allows access to the following parameters:

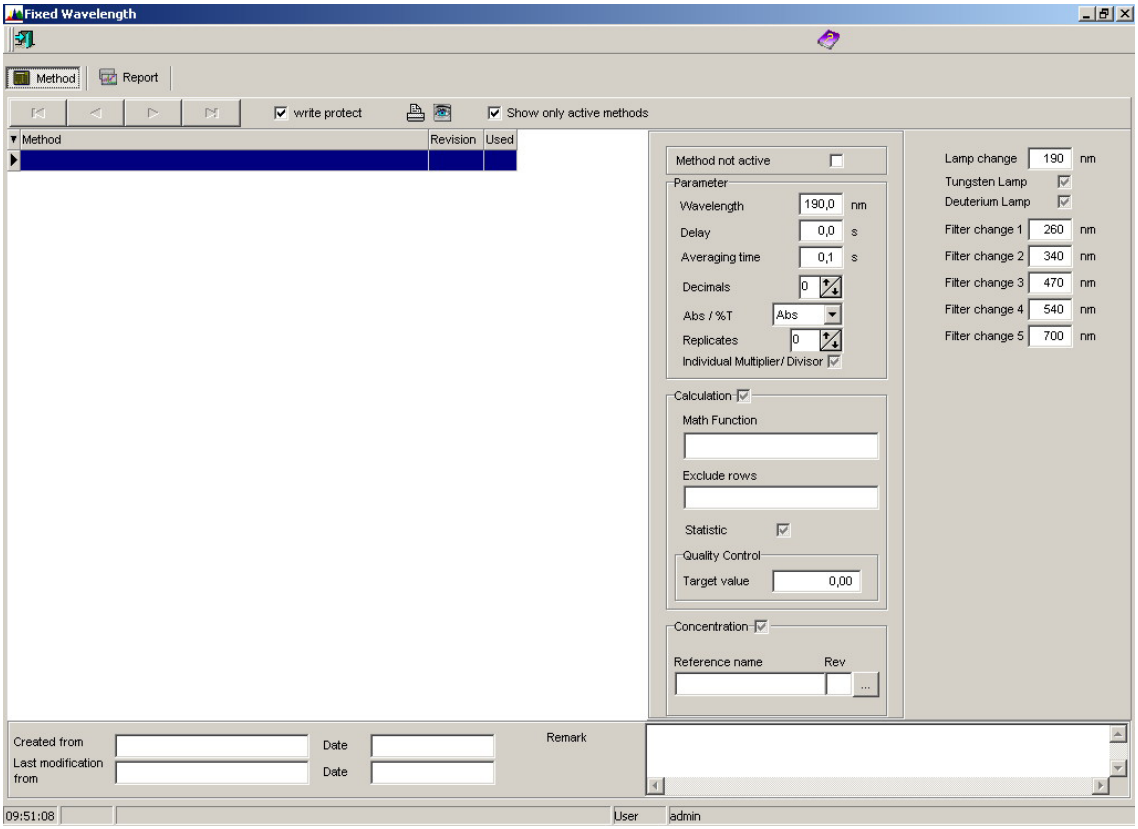


Factor The factor can be used to calculate concentrations or other values if the response of the substance measured is known. In this case use of a calibration file would not be necessary.

View These checkboxes permit toggling between absorbance and transmission values for the display of the acquired data. The data is always saved according to the definitions in the method independent of this setting.

2.4.1.3. The Method in Fixed Wavelength

Click on the *Method* button in the upper left corner to open the *Method* window:



The left-hand window contains a list of all existing methods including revisions and an indication of whether they have been used already or not.

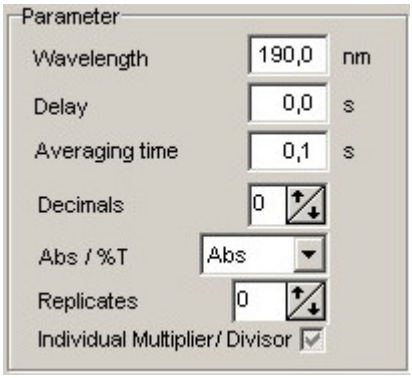
Caution: *If measurements have been used, the method will be locked and can no longer be changed. However, they can be used for later measurements or modified with revision control. Such methods are indicated by a " * " in the " used " column list.*

A new method can be created from within the method section by using the '+' button. In order to do this it is first necessary to uncheck the write-protect checkbox.

The system will first prompt for name under which the new method will be saved. Once this has been defined all other parameters can be entered.

2.4.1.3.1. Acquisition parameters

Method not active Inactivate, and thus hide the current *Method* by checking this box.



Wavelength Defines the wavelength to be used for the measurement.

Delay time The instrument will wait for the selected delay time after the MEASURE key is pressed to start the actual measurement.

Averaging time Defines the time the instrument uses to collect data for calculation of a mean value for one reading. A long averaging time is useful to reduce noise when measuring at high absorbance values.

Decimals Defines the amount of decimals for the measurement values.

Abs / %T Selection permits definition of the mode to be used. The user can select between either absorbance or transmission.

Replicates Defines the number of acquisitions per sample to determine the resulting mean.
E.g.: Replicates = 0 : only one acquisition per sample
Replicates = 1 : two acquisitions per sample

Individual Multiplier/Divisor By checking this box, a separate dilution factor (multiplier) and weight factor (divisor) can be defined for each sample.

2.4.1.3.2. Common Parameters

The right-hand panel contains common parameters, which are required for every system and user method. They will be stored and recalled along with all other parameters.

Lamp change This parameter defines the lamp change wavelength. The deuterium lamp is used for all wavelengths below the lamp change wavelength. The tungsten halogen lamp is used for all wavelengths above the lamp change wavelength.

Tungsten lamp When checked the tungsten lamp will be switched on and used according to the setting for the lamp change.

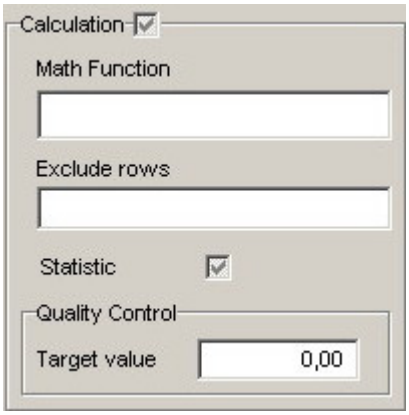
Deuterium lamp When checked the deuterium lamp will be switched on and used according to the setting for the lamp change.

Filter change (1-5) This parameter defines the wavelength used to switch the filter.

Bandwidth Selects the spectral bandwidth of the spectrophotometer.

Cell changer Defines the operating mode of the cell changer (if fitted).

2.4.1.3.3. Calculation



Calculation Deactivate *Calculation* for normal acquisitions without any special calculation. Activate *Calculation* for special calculations defined under *Math Function*.

Math Function This function depends on the grid of absorbance values. Enter the calculation desired.
Examples: ((A1-A2)-(A4-A3))*F ; ((A1-A2)-(A1,1-A2,1))*F

Table Matrix Example I:

Abs 1	Abs 2	Abs 3	Abs 4	Result
A1	A2	A3	A4	V

Table Matrix Example II:

Abs 1	Abs 2	Abs 3	Result
A1,1	A2,1	A3,1	W
A1,2	A2,2	A3,2	X
A1,3	A2,3	A3,3	Y
A1,4	A2,4	A3,4	Z

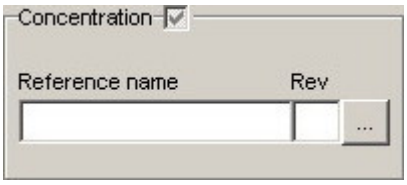
The first number indicates the different measurements of one sample, the second number indicates the sample number. E.g.: A2,1 is the first replicate of the first sample, A1,2 is the first measured value of sample no. 2.
F = factor given with the acquisition window
Other operators (*,/,+,sqr,...) may be entered.

Exclude rows Enter the rows to be excluded. The calculation of results (mean, std dev,...) will not use these rows for calculation.

Target value This is a value for the statistics window. The deviation will be calculated with the mean value and the target value.

Note: *Calculation and Concentration checkboxes cannot both be ticked at the same time. An error message will be shown during saving of the method.*

2.4.1.3.4. Concentration



If the *Concentration* checkbox is ticked, the system will use the defined calibration reference for the calculation of the concentration values based on the results of the measurement.
By clicking the "..."-button next to the *Rev* Box, you can select the calibration file to be used. The boxes show the *Reference name* of the selected file and its revision number (*Rev*).

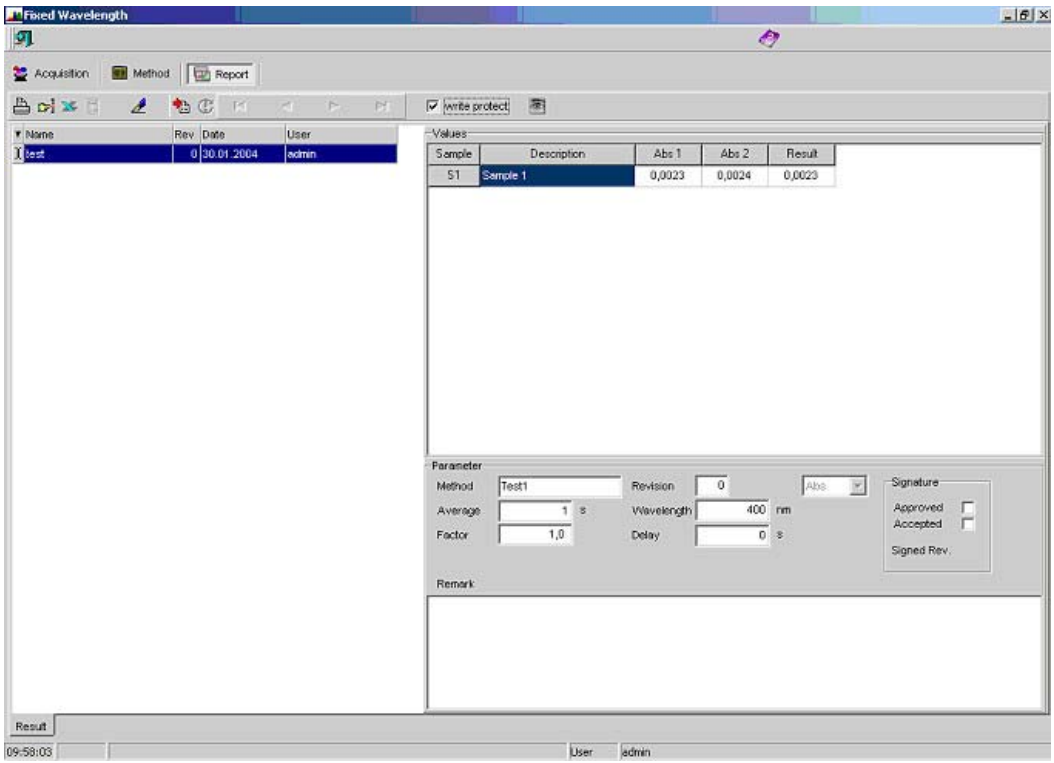
Note: Calculation and Concentration checkboxes cannot both be ticked at the same time. An error message will be shown during saving of the method.

2.4.1.3.5. Audit Trail in Fixed Wavelength Method

Click on the Audit Trail icon to view the audit trail window for the method.

2.4.1.4. The Report Screen in Fixed Wavelength

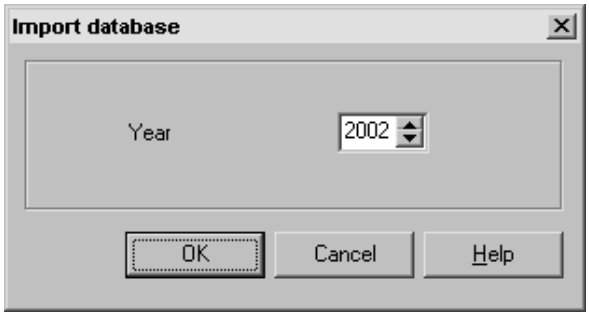
Click on the *Report* button in the upper left corner to open the *Report* window:



The left-hand window contains a list of all available reports, the right-hand window contains the results in the upper section and the main parameters for the measurement in the lower part. Each report can be viewed by scrolling through the left-hand list.

2.4.1.4.1. Printing

Click on the *Print* icon to obtain a print preview of the selected report, which will always contain all measurements. The report can be printed by clicking on the *Print* icon on the preview page.



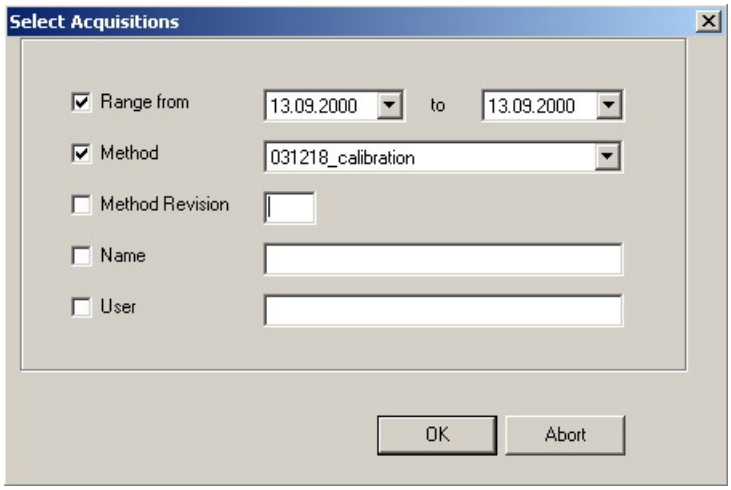
2.4.1.4.2. Importing a report from the database

Click on the *Import* icon to access earlier reports in the extracted database. A dialogue window for selection of the database will be opened:

2.4.1.4.3. Filtering the report list

The report list in the left window will become very long with time and it may be necessary to filter the list so that only those files of interest to a user are actually shown. This is carried out using the *Select Report* icon.

Click on the *Select Report* icon and a dialogue window appears, which allows selection of a view by date, method, user or name:



The appropriate checkbox must be checked and, where applicable, either a date or name selected. Clicking on *OK* will cause only those reports which satisfy all selected criteria to be shown in the list of available reports.

2.4.1.4.4. Audit Trail in Fixed Wavelength Report

Click on the *Audit Trail* icon to view the audit trail window for the report.

2.4.1.5. Calculations in Fixed Wavelength

Fixed Wavelength contains four basic calculation methods for final result determination:

- Linear regression
- Quadratic regression
- Blank
- Factor

In *Fixed Wavelength* the *Blank* and *Factor* calculations are executed automatically without the need to create a calibration file:

Blank The measured values for sample blank is subtracted from the measured value of each sample measured.

Factor The actual value obtained from the measurement is always multiplied by the factor parameter. This is accessible by clicking on the *Parameter* tab in the acquisition screen.

The actual calculation is based on the following formula:

$$R = F * (VM_{sample} - VM_{blank})$$

Where R = Result, F = Factor and VM represents the measured values obtained for sample and blank respectively.

Recalculation after, for example, changing the factor value is possible at any time by clicking on the *Calculator* icon.

2.4.1.6. Concentration in Fixed Wavelength

In simple cases the *Result* obtained above can be used as a concentration value if the *Factor* has been defined and zero concentration corresponds to zero absorbance.

Using the calibration function, it is possible to calculate concentration values based on a previously determined calibration curve. This method offers the advantage that any absorbance offset is compensated for and that the final result is given in the desired units in the report print-outs.

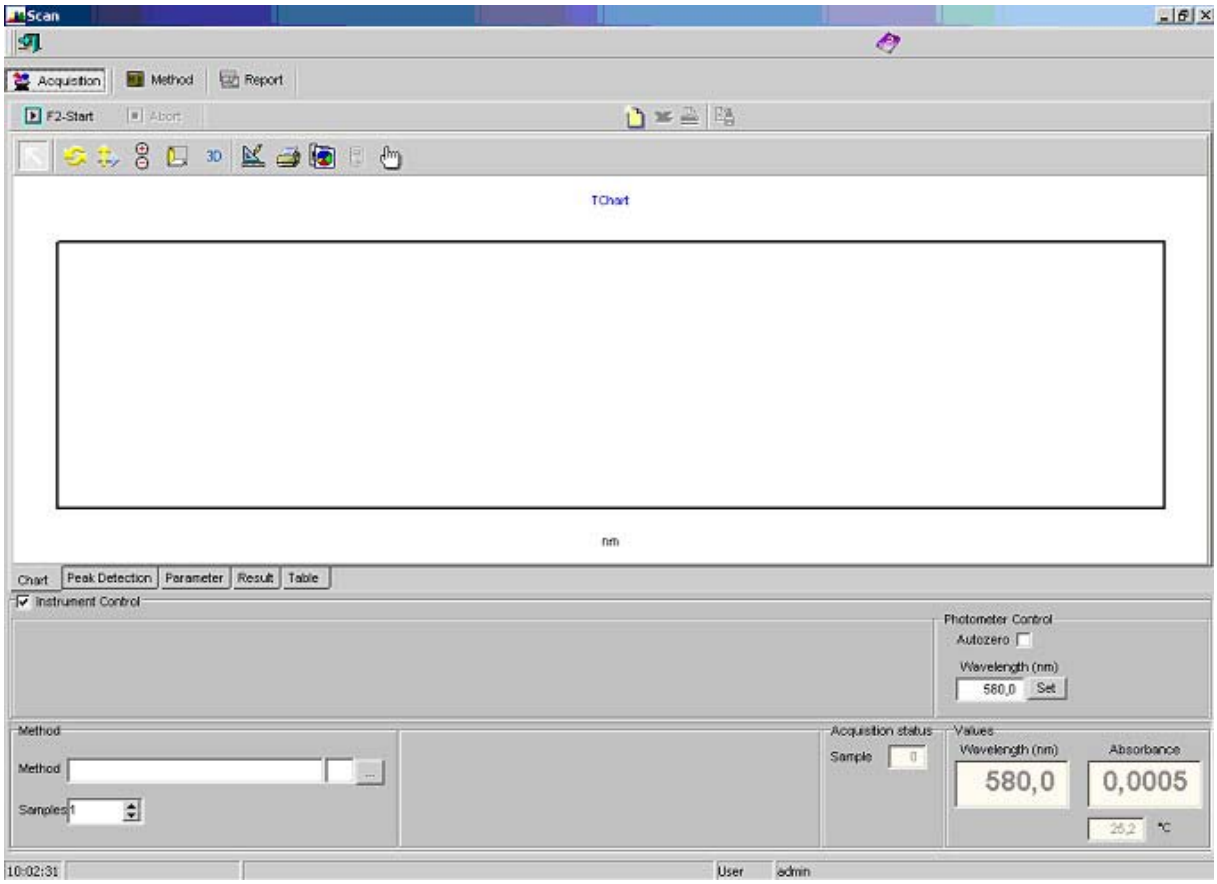
The calibration uses the value obtained for the *Result* (see above) and converts this value to a corresponding concentration value in units, which are defined as part of the calibration file.

A more detailed description of the *Calibration* function is given in a separate section within this document.

2.4.2. Wavelength Scan

2.4.2.1. The Acquisition Screen in Wavelength Scan

Select **"Wavelength Scan"** from the main menu to obtain the following display:



This is the acquisition window from which all measurements are started. In this window the following parameters must be selected before starting a measurement:

- Method to be used for the acquisition. The method contains all parameters necessary for the execution of the measurement.
- Numbers of samples to be measured.
- *Autozero* at start of measurement.

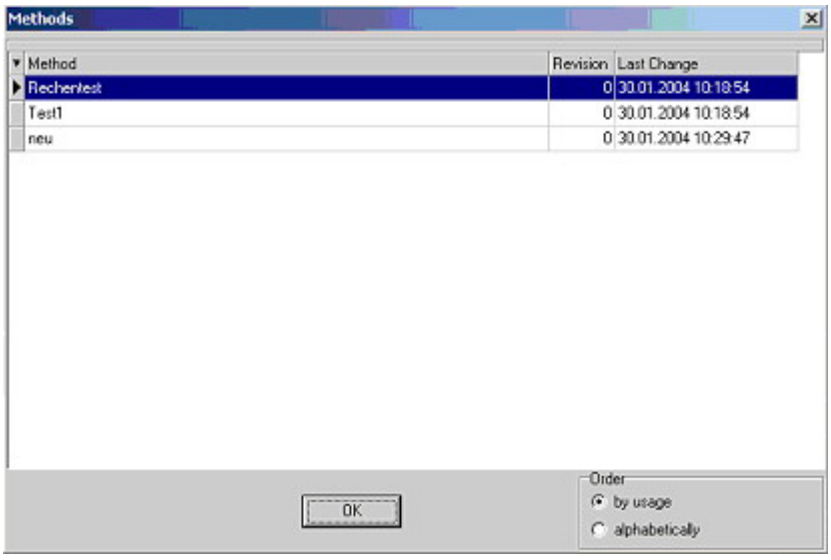
2.4.2.1.1. Run parameters

The run parameters are entered in the “Method” panel and in the “Photometer control” panel:

Samples Defines the number of samples to be analysed.

Autozero Defines whether an autozero should be executed prior to the start of a measurement.

Method The method box contains the name of the method and, directly adjacent, the actual revision number of that method. The method is selected from a separate window which opened by clicking on the button adjacent to the revision box:



This window contains a list of all available methods including all revisions of the method and the date of last modification. Selection is made by highlighting the required line and then clicking on *OK*.
The order of Methods may be displayed by usage or alphabetically.

Wavelength A certain wavelength may be chosen manually and set immediately in order to allow rapid monitoring of the unit.

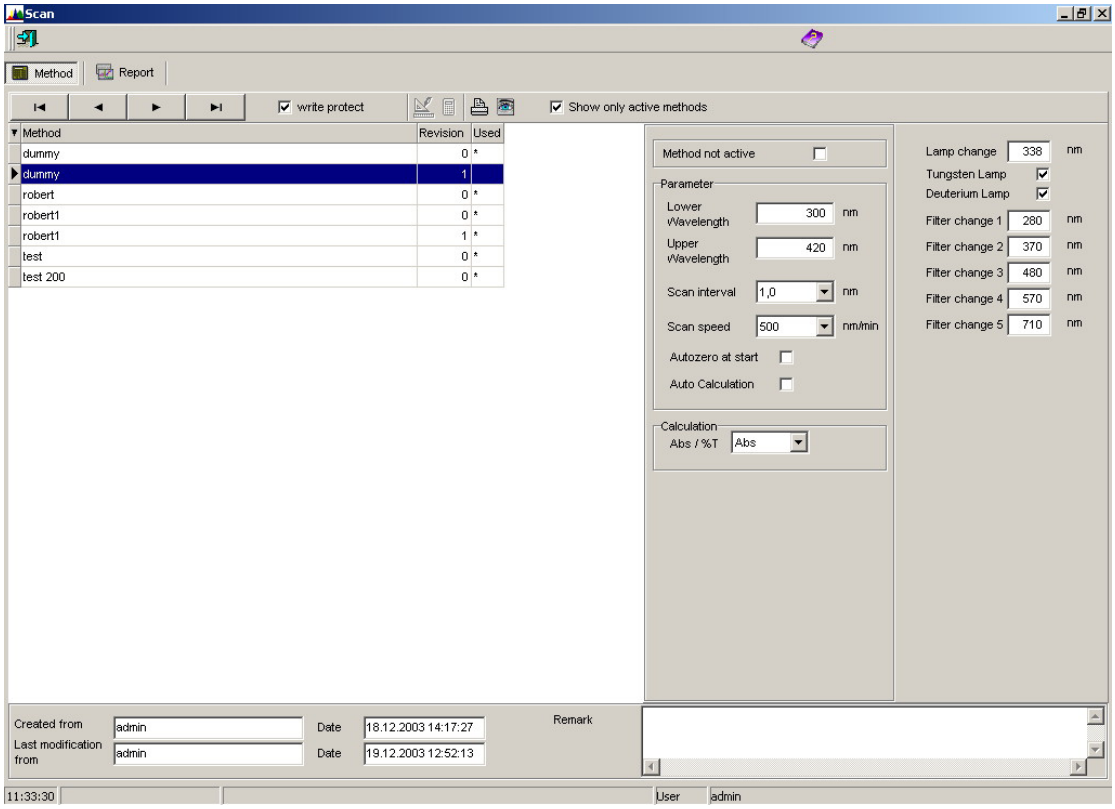
2.4.2.1.2. System Status

The lower right section of the display contains the actual status of the system and displays the following parameters:

- Current sample being measured.
- Actual wavelength.
- Actual absorbance value.
- Temperature (where applicable).

2.4.2.2. The Method in Wavelength Scan

Click on the *Method* button in the upper left corner to open the *Method* window:



The left-hand window contains a list of all existing methods including revisions and an indication of whether they have been used already or not.

Caution: *If measurements have been used, the method will be locked and can no longer be changed. However, they can be used for later measurements or modified with revision control. Such methods are indicated by a " * " in the " used " column list.*

A new method can be created from within the method section by using the '+' button. In order to do this it is first necessary to uncheck the write-protect checkbox.

The system will first prompt for name under which the new method will be saved. Once this has been defined all other parameters can then be entered.

2.4.2.2.1. Acquisition parameters

Method not active Inactivate, and thus hide the current *Method* by checking this box.

Lower Wavelength Defines the lower wavelength for the wavelength range to be used for the measurement.

Upper Wavelength Defines the upper wavelength for the wavelength range to be used for the measurement.

Scan Interval This parameter (also called sampling interval in other instruments) defines the wavelength step between two measured data points.

Scan Speed Defines the wavelength drive speed to be used for the measurement. Scanning speeds can be selected between 5 and 5000 nm/min. If you choose dynamic scan speed, the instrument will automatically optimise the scan speed to suit the slope of your sample.

Autozero If checked, an autozero will be made for each sample beforestarting the scan.

Auto Calculation If checked, the calculation for peak detection, smoothing etc. starts automatically after acquisition using the defined parameters.

2.4.2.2.2. Common Parameters

The right-hand panel contains common parameters, which are required for every system and user method. They will be stored and recalled along with all other parameters.

Lamp change This parameter defines the lamp change wavelength. The deuterium lamp is used for all wavelengths below the lamp change wavelength. The tungsten halogen lamp is used for all wavelengths above the lamp change wavelength.

Tungsten lamp When checked, the tungsten lamp will be switched on and used according to the setting for the lamp change.

Deuterium lamp When checked, the deuterium lamp will be switched on and used according to the setting for the lamp change.

Filter change (1-5) This parameter defines the wavelength used to switch the filter.

Bandwidth Selects the spectral bandwidth of the spectrophotometer.

Cell changer Defines the operating mode of the cell changer (if fitted).

2.4.2.2.3. Calculation

The calculation selection permits definition of the mode of calculation to be used. The user can select between either absorbance or transmission.

2.4.2.2.4. Curve Parameters in the Wavelength Scan Method

Opens an edit dialogue for defining curve parameters and related formatting.

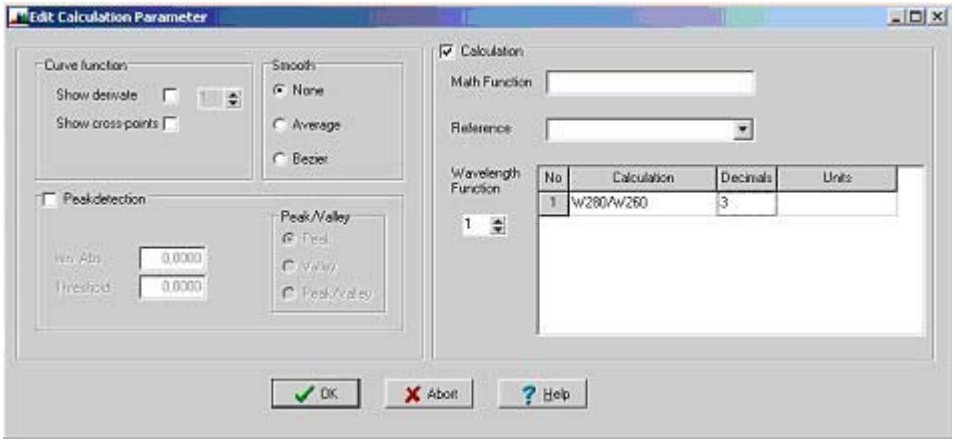
In *Wavelength Scan* the curve parameters can be linked to a method and then define the appearance and properties of the curve such as colours, overlay format, scaling etc.

Functions defined here will be included and stored with the method and thus used for any acquisition executed utilising that method.

Formatting options using this function are described in a separate section of this document.

2.4.2.2.5. Calculation Parameters in the Wavelength Scan Method

Click on this icon to open the calculation dialogue window for the method:



By activating the *Calculation* box, a mathematical function or/and a wavelength function may be implemented.

The *Math Function* may be defined with or without a reference file.
E.g.: S-R Subtract reference from all samples
S+R Add reference to all samples
S*1.2 Multiply all samples with 1.2 (Format 1.2 or 1,2 depends on windows)

To use the *Wavelength Function*, choose the number of functions and then enter the wavelength and a mathematical function to have a calculated result.
E.g.: W280/W260
W250*1.2
W300-W350
Nested functions are possible, too.

Some of the calculation functions shown in the dialogue above are described in more detail in the section on Calculation within this document. Functions defined above will be included and stored with the method and thus used for any acquisition executed utilising that method.

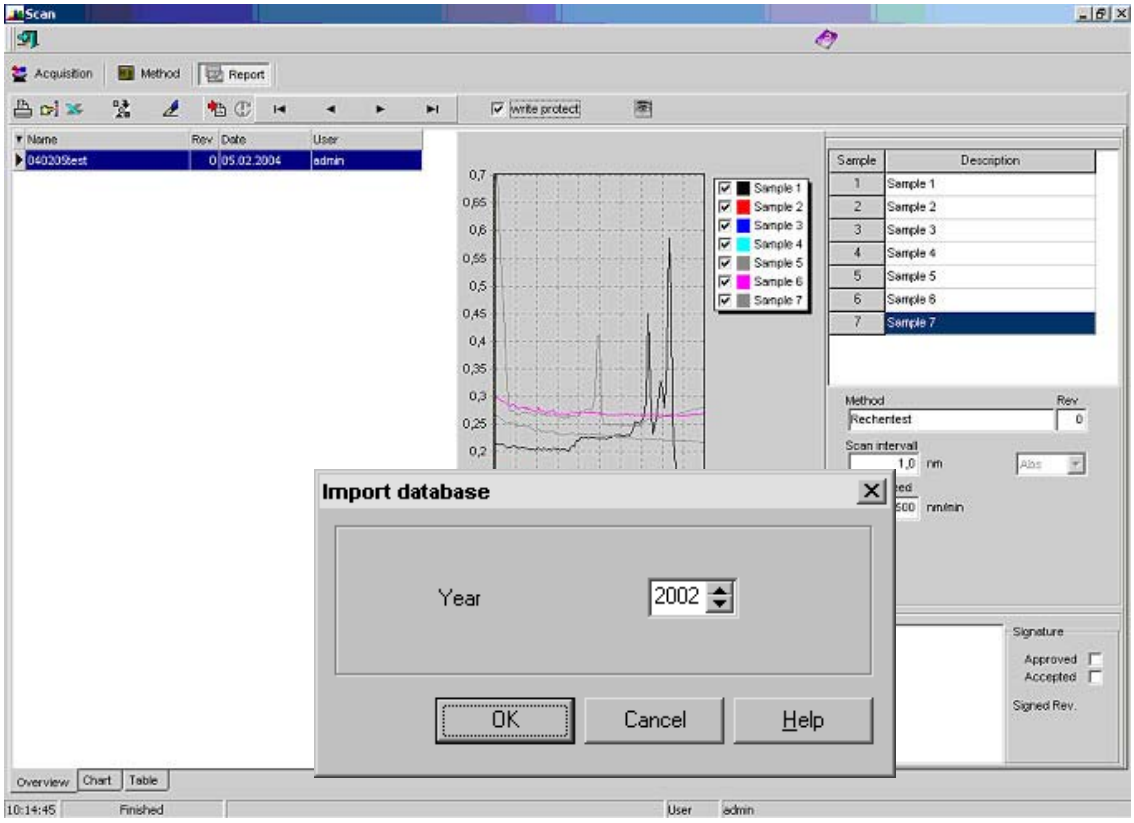
2.4.2.2.6. *Audit Trail in Wavelength Scan Method*

Click on the *Audit Trail* icon to view the audit trail window for the method.

2.4.2.3. The Report Screens in Wavelength Scan

2.4.2.3.1. The "Overview" Report Screen

Click on the *Report* button in the upper left corner to open the *Report* window:



The display obtained is the “Overview” screen, clicking on the “Chart” tab will display the chart as the main item which can be manipulated or edited as required.

The left-hand window contains a list of all available reports, the right-hand window contains the results in the upper section and the main parameters for the measurement in the lower part. Each report can be viewed by scrolling through the left-hand list.

2.4.2.3.2. Printing

Click on the *Print* icon to obtain a print preview of the selected report, which will always contain all measurements. The report can be printed by clicking on the *Print* icon on the preview page.

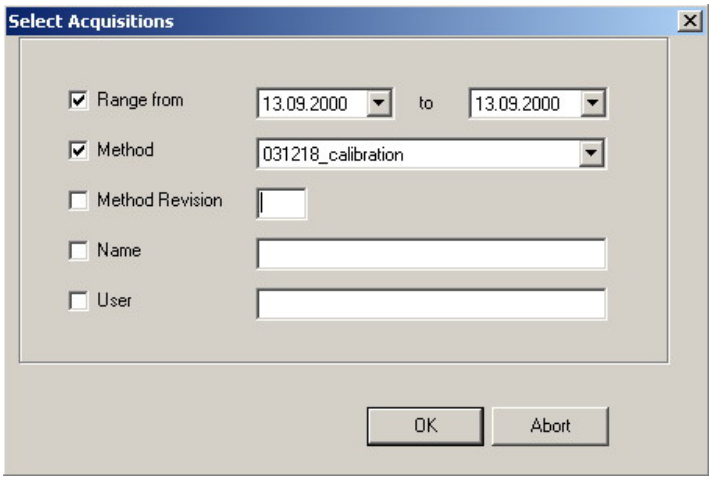
2.4.2.3.3. Importing a report from the database

Click on the *Import* icon to access earlier reports in the archived database. A dialogue window for selection of the database will be opened:

2.4.2.3.4. Filtering the report list

The report list in the left window will become very long with time and it may be necessary to filter the list so that only those files of interest to a user are actually shown. This is carried out using the *Select Report* icon.

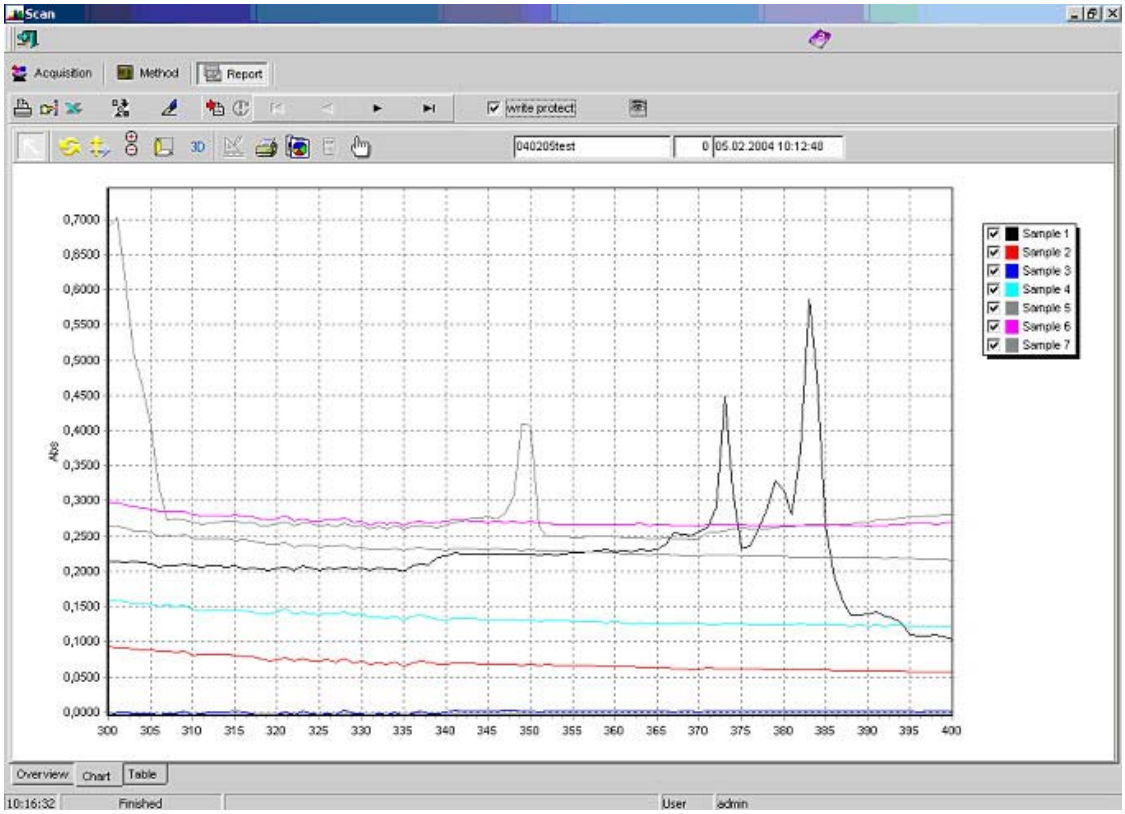
Click on the *Select Report* icon and a dialogue window appears, which allows selection of a view by date, method, user or name:



The appropriate checkboxes must be checked and, where applicable, either a date or name entered. Clicking on *OK* will cause only those reports which satisfy all selected criteria to be shown in the list of available reports.

2.4.2.3.5. The "Chart" Report Screen

Clicking on the "Chart" tab will open a new screen containing the curve in a form which can be edited:



Curves may be displayed as overlays, individual curves can be removed from the overlay if required by clicking the checkboxes shown as part of the legend on the right of the curve.

Navigation arrows are available to move between the various reports contained in the list without the need to return to the *Overview* screen.

The name of the currently displayed curve set including the revision is shown in the box display immediately above the curve display.

In *Chart* mode a range of new functions is available to the user for manipulating the presentation and properties of the current curve.

2.4.2.3.6. "Chart" Report Screen Functions

A graphics toolbar is available within the *Chart report screen*:

The use of the icons in the graphics toolbar allow direct manual manipulation of the currently displayed chart. The function of the individual icons is described briefly below:

Shows position of values on X- and Y-axis and allows to manually pick peaks and to add, edit or delete comments.

Opens the calculation dialogue window.

Exports a curve to the *Windows clipboard* for further processing.

Prints the curve as a single sheet report. Formatting of the report is described in a separate section of this document dealing with curve format.

Opens the edit dialogue for formatting functions. See the separate section of this document dealing with curve format for more details.

Converts chart format to a 3D display. The icon functions as a toggle switch between a 2D and 3D display.

Click on this icon to control the depth of the 3D display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Double function icon allowing zooming of the complete curve.

Click on this icon to move the complete curve display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Click on this icon to rotate the complete curve display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Clicking on this icon will return the function of the mouse cursor to normal thus allowing use of the normal zooming functions etc. in 3D displays.

2.4.2.3.7. Audit Trail in Wavelength Scan Report

Click on the *Audit Trail* icon to view the audit trail window for the report.

2.4.2.4. Calculations in Wavelength Scan

The curve calculation modes are generally embedded in the method and are described above and in detail in the *Calculation* section.

Recalculation after, for example, changing a *Peak Detection* parameter is possible at any time by clicking on the *Calculator* icon followed by election of the parameter within the dialogue window.

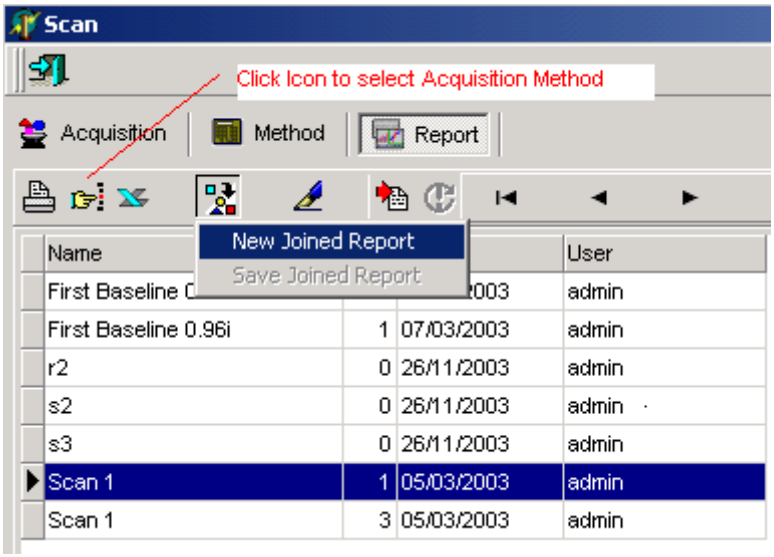
2.4.2.5. Peak Detection

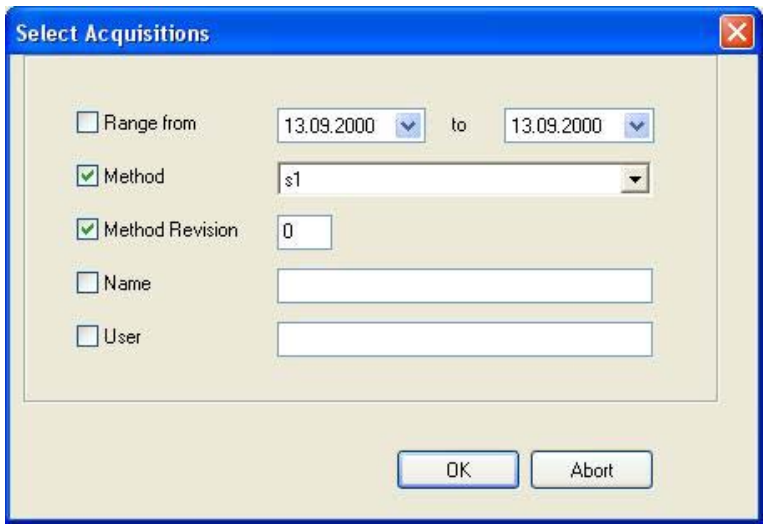
Clicking on the peak detection tab will show the list of wavelength and absorbance values for the detected peaks.

2.4.2.6. Joined Reports

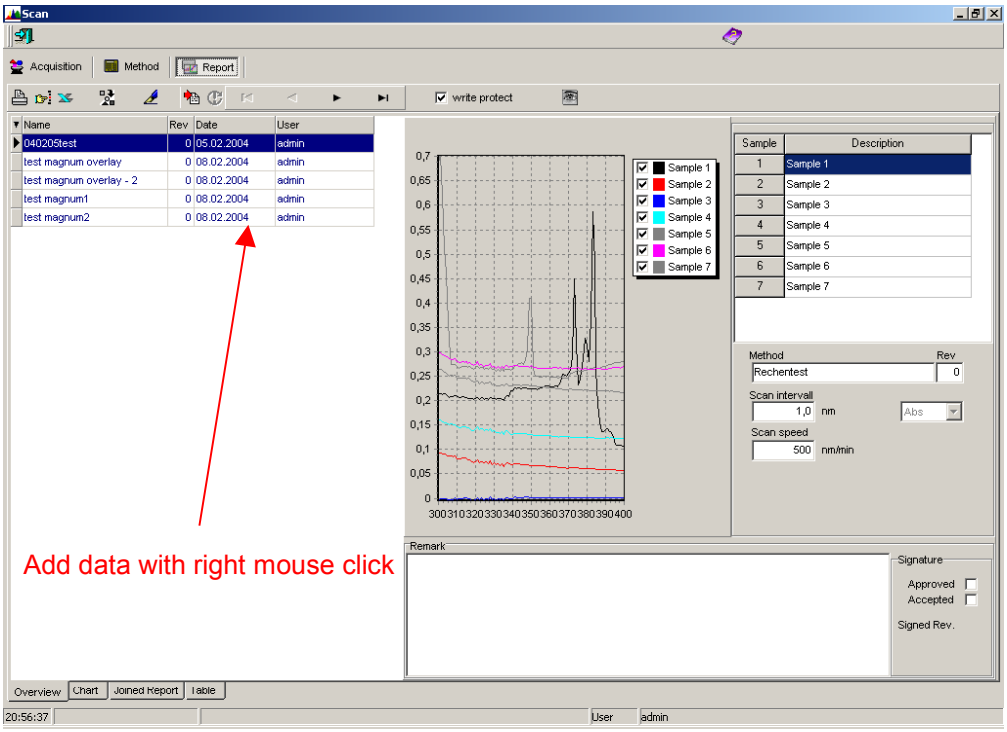
The “Joined Report” option offers the possibility the overlay of spectra from different runs of the same method after the reports have been saved.

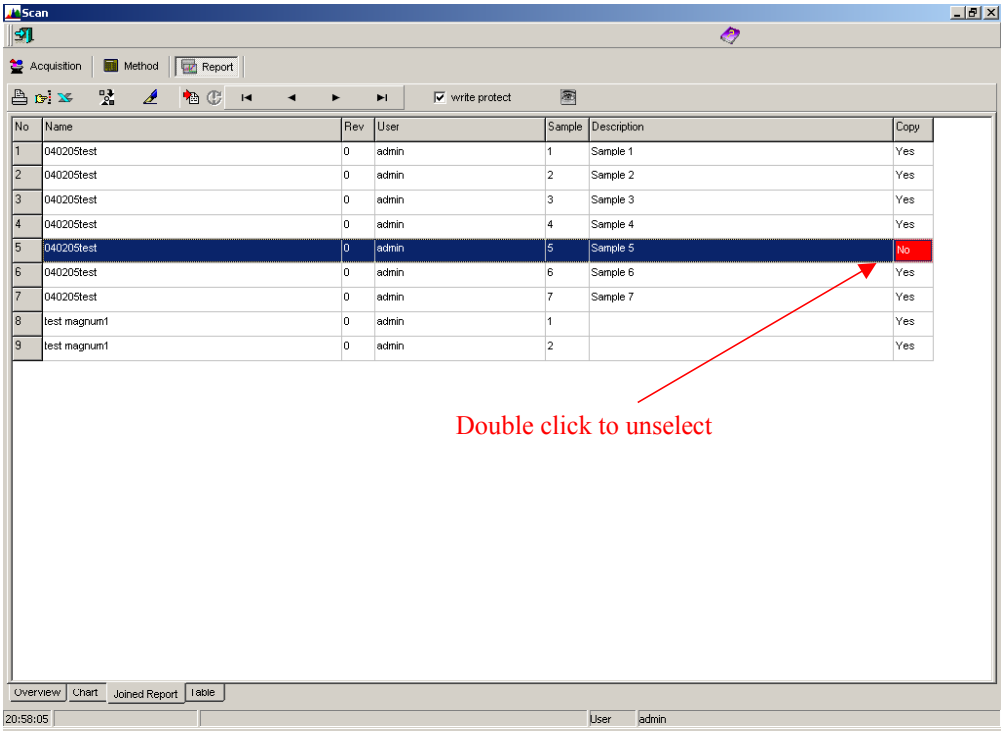
To use the Join Report Option click on “New Joined Report” icon and then choose the method that you want to join your reports from. Please not that only data acquired with identical method and revision of method can be overlayed and make sure that select and enter both values.





Select dataset from the Overview List and then add the file by using the right mouse button. The selection of datasets can be monitored in the card “Joined Report” during the process. After the completed selection of your datasets save the created Joined Report File.
The overlay is saved as a normal report, so that all mathematical and graphical functions are available.

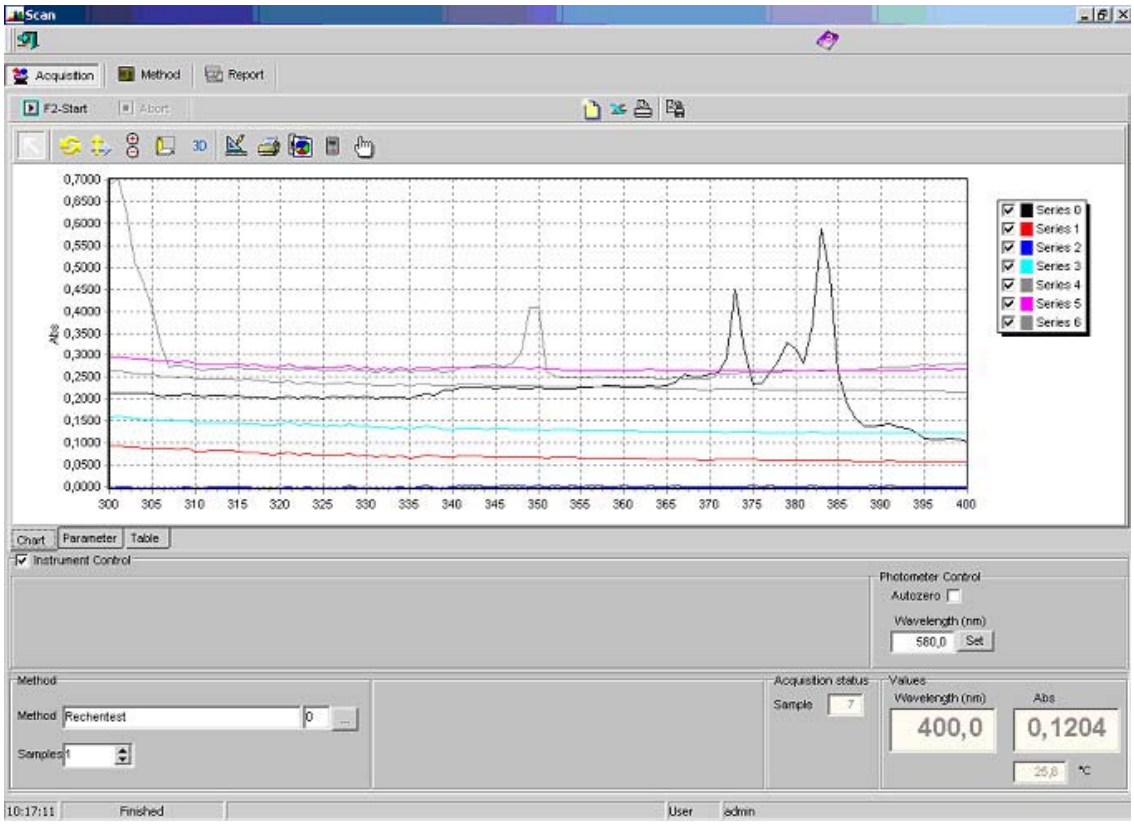




2.4.2.7. Wavelength Scan Measurement Example

Scanning measurement of one blank and five samples using the cell changer.

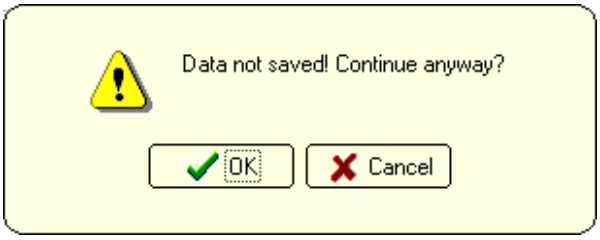
Select the method to be used and set the number of samples to 6. Insert the samples into the cell changer and start the measurement by pressing the *Start* button. The measured curves are displayed in real time during acquisition. A 3D display (see below) may be used to give better clarity if the curves are very similar for each sample. The final window will look similarly like this:



Note: *If you are not using a cell changer, you will be prompted for the next sample after each sample has been measured. The final appearance of the screen remains unchanged.*

Individual curves may be removed from the overlay display by clicking the checkboxes in the legend on the right of the curve.

If you repeat the measurement you will always measure the selected number of samples (6 in our example) until you change the *Samples* parameter. The system will prompt if the previously run sample data has not been saved beforestarting a new run:



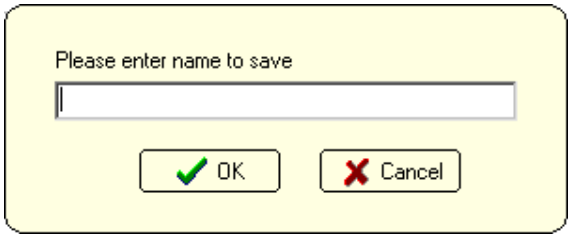
Click on *OK* to start the next acquisition run or on *Cancel* to return to the original data set.

Printing

Click on the *Print* icon to obtain a preview of the printed report, which will always contain all measurements. If the result is acceptable the report can be printed by clicking on the *Print* icon on the preview page.

Saving

Click on the *Save* icon and the system will prompt for a file name:

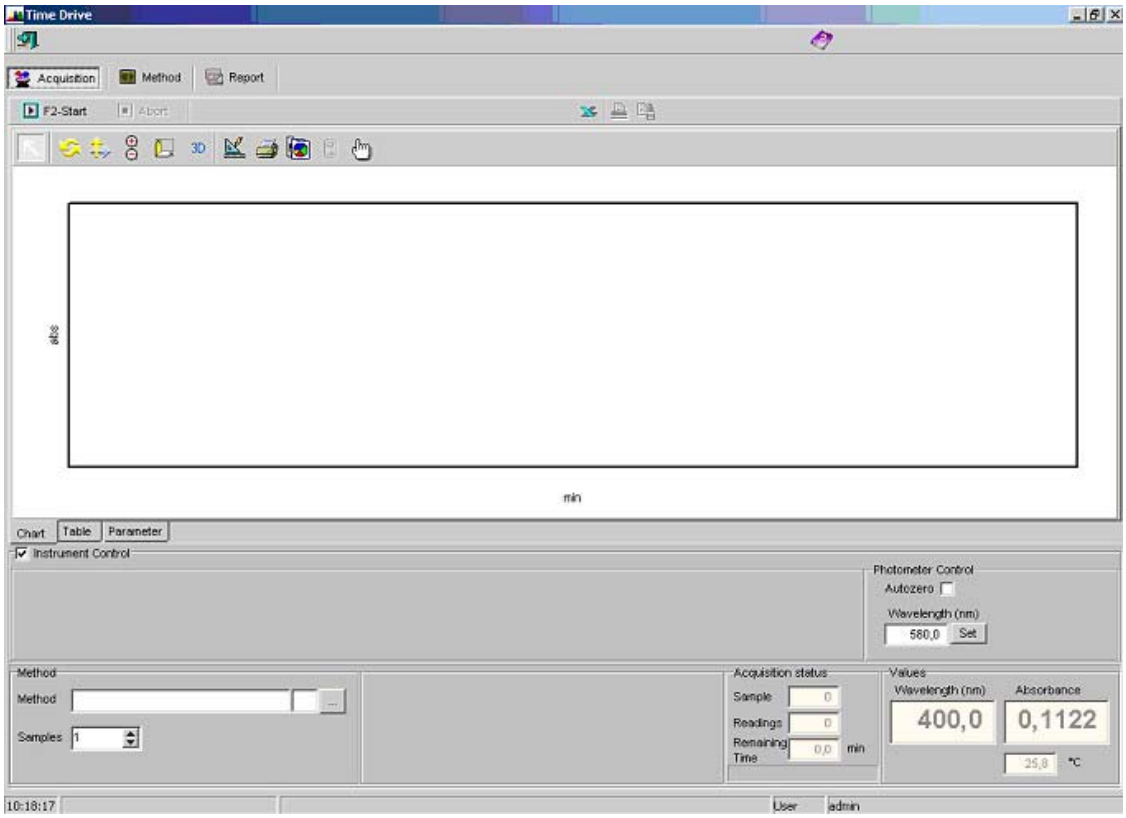


Enter the file name and click on *OK*.

2.4.3. Time Drive

2.4.3.1. The Acquisition Screen in Time Drive

Select **"Time Drive"** from the main menu to obtain the following display:



This is the acquisition window from which all measurements are started. In this window the following parameters must be selected before starting a measurement:

- Method to be used for the acquisition. The method contains all parameters necessary for the execution of the measurement.
- Numbers of samples to be measured.
- *Autozero* at start of measurement.

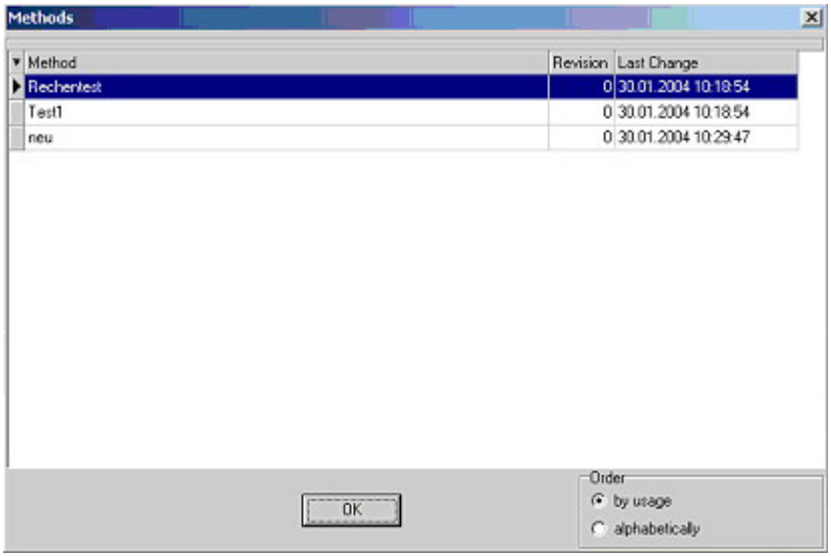
2.4.3.1.1. Run parameters

The run parameters are entered in the "Method" panel and in the "Photometer control" panel:

Samples Defines the number of samples to be analysed.

Autozero Defines whether an autozero should be executed before starting a measurement.

Method The method box contains the name of the method and, directly adjacent, the actual revision number of that method. The method is selected from a separate window which is opened by clicking on the button adjacent to the revision box:



This window contains a list of all available methods including all revisions of the method and the date of last modification. Selection is made by highlighting the required line and then clicking on OK.
The order of Methods may be displayed by usage or alphabetically.

Wavelength A certain wavelength may be chosen manually and set immediately in order to allow rapid monitoring of the unit.

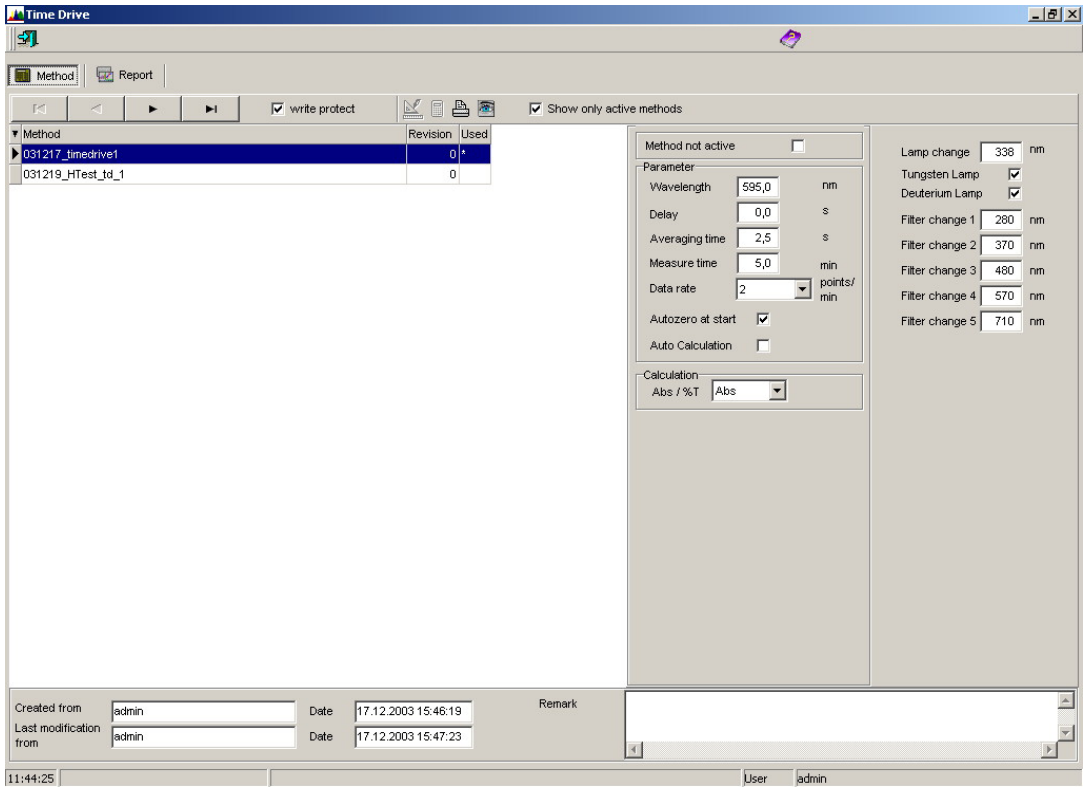
2.4.3.1.2. System Status

The lower right section of the display contains the actual status of the system and displays the following parameters:

- Current sample being measured.
- No. of Readings
- Remaining Time (also as progress bar)
- Actual wavelength.
- Actual absorbance value.
- Temperature (where applicable).

2.4.3.2. The Method in Time Drive

Click on the *Method* button in the upper left corner to open the *Method* window:



The left-hand window contains a list of all existing methods including revisions and an indication of whether they have been used already or not.

Caution: *If measurements have been used, the method will be locked and can no longer be changed. However, they can be used for later measurements or modified with revision control. Such methods are indicated by a " * " in the " used " column list.*

A new method can be created from within the method section by using the '+' button. In order to do this it is necessary to uncheck the write-protect checkbox.

The system will first prompt for name under which the new method will be saved. Once this has been defined all other parameters can be entered.

2.4.3.2.1. Acquisition parameters

Method not active Inactivate, and thus hide the current *Method* by checking this box.

Wavelength Defines the wavelength to be used for the measurement.

Delay time The instrument will wait for the selected delay time after the MEASURE key is pressed to start the actual measurement.

Averaging time Defines the time the instrument uses to collect data for calculation of a mean value for one reading. A long averaging time is useful to reduce noise when measuring at high absorbance values.

Measure time Defines the actual duration of the measurement in minutes.

Sampling rate Defines the number of data points per minute for the measurement.

Autozero at start Defines whether an autozero is to be executed beforeeach sample run.

Auto Calculation If checked, the calculation for peak detection, smoothing etc. starts automatically after acquisition using the defined parameters.

Calculation mode Calculation and curve portrayal can be in either *Absorbance* or *Transmission* units.

2.4.3.2.2. Common Parameters

The right-hand panel contains common parameters, which are required for every system and user method. They will be stored and recalled along with all other parameters.

Lamp change This parameter defines the lamp change wavelength. The deuterium lamp is used for all wavelengths below the lamp change wavelength. The tungsten halogen lamp is used for all wavelengths above the lamp change wavelength.

Tungsten lamp When checked, the tungsten lamp will be switched on and used according to the setting for the lamp change.

Deuterium lamp When checked, the deuterium lamp will be switched on and used according to the setting for the lamp change.

Filter change (1-5) This parameter defines the wavelength used to switch the filter.

Bandwidth Selects the spectral bandwidth of the spectrophotometer.

Cell changer Defines the operating mode of the cell changer (if fitted).

2.4.3.2.3. Calculation

The calculation selection permits definition of the mode of calculation to be used. The user can select between either absorbance or transmission.

2.4.3.2.4. Curve Parameters in the Time Drive Method

Opens an edit dialogue for defining curve parameters and related formatting.

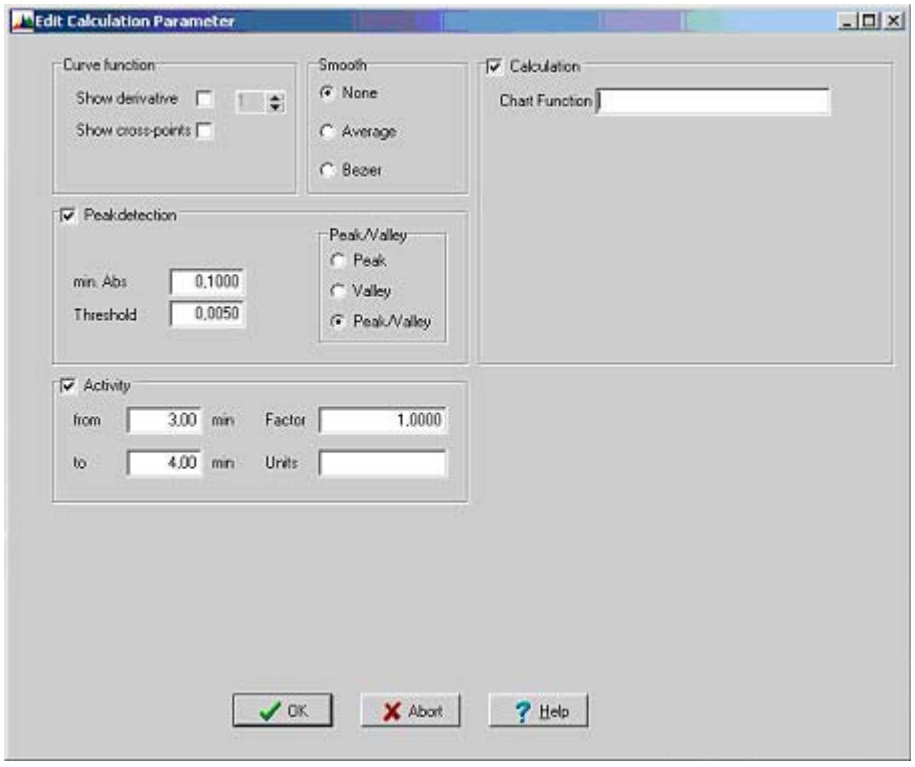
In *Time Drive* the curve parameters can be linked to a method and then define the appearance and properties of the curve such as colours, overlay format, scaling etc.

Functions defined here will be included and stored with the method and thus used for any acquisition executed utilising that method.

Formatting options using this function are described in a separate section in this document.

2.4.3.2.5. Calculation Parameters in the Time Drive Method

Click on this icon to open the calculation dialogue window for the method:

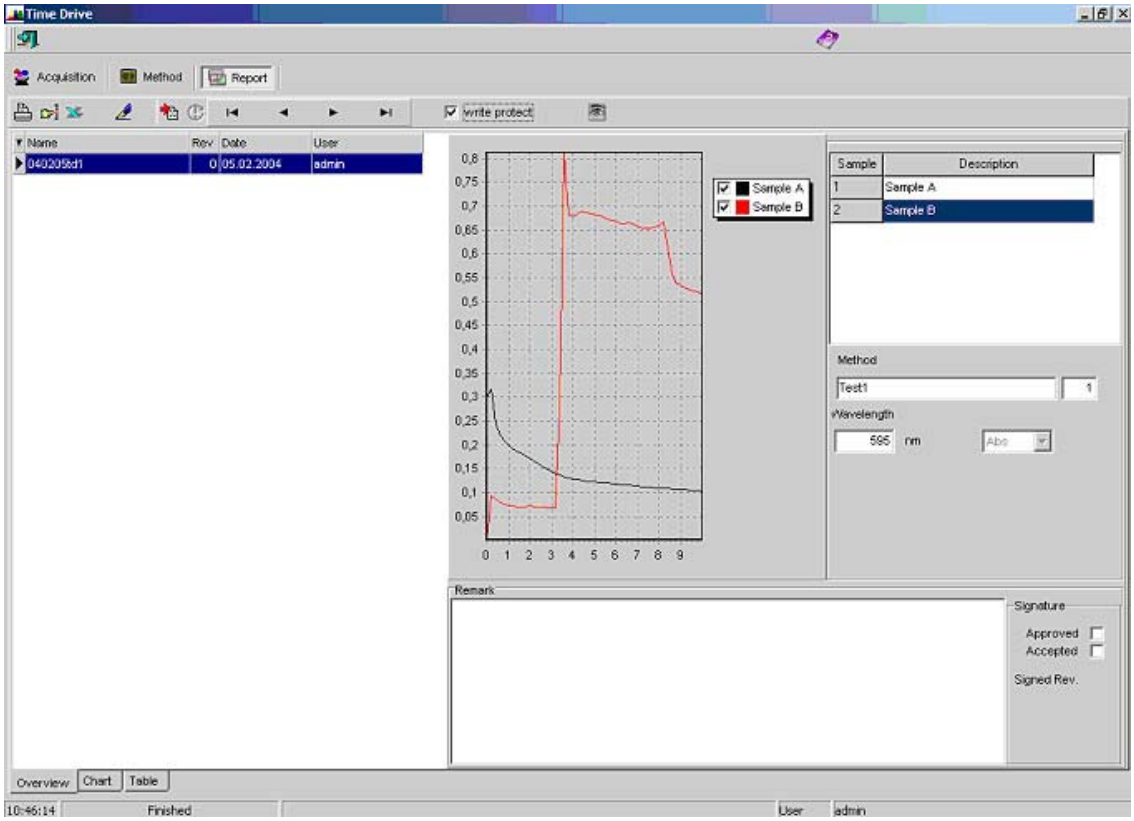


The calculation functions shown in the dialogue above are described in more detail in the section on *Calculation* within this document. Functions defined above will be included and stored with the method and thus used for any acquisition executed utilising that method.

2.4.3.3. The Report Screens in Time Drive

2.4.3.3.1. The "Overview" Report Screen

Click on the *Report* button in the upper left corner to open the *Report* window:



The display obtained is the "Overview" screen, clicking on the "Chart" tab will display the chart as the main item and this can be manipulated or edited as required.

The tabs for *Activity* and *Peak Detection* show a display in table form for the respective parameters

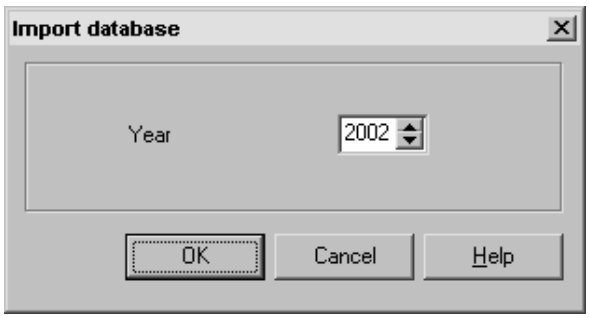
The left-hand window contains a list of all available reports, the right-hand window contains the results in the upper section and the main parameters for the measurement in the lower part. Each report can be viewed by scrolling through the left-hand list.

2.4.3.3.2. Printing

Click on the *Print* icon to obtain a print preview of the selected report, which will always contain all measurements. The report can be printed by clicking on the *Print* icon on the preview page.

2.4.3.3.3. Importing a report from the database

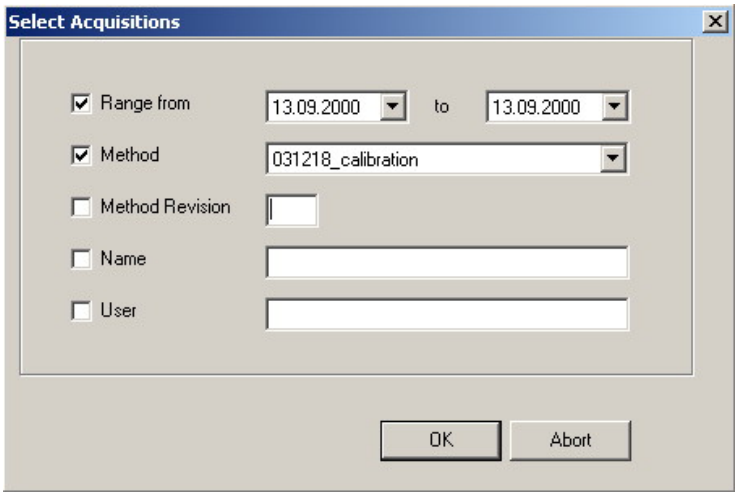
Click on the import icon to access earlier reports in the archived database. A dialogue window for selection of the database will be opened:



2.4.3.3.4. Filtering the report list

The report list in the left window will become very long with time and it may be necessary to filter the list so that only files of interest are shown to a user. This is carried out using the *Select Report* icon.

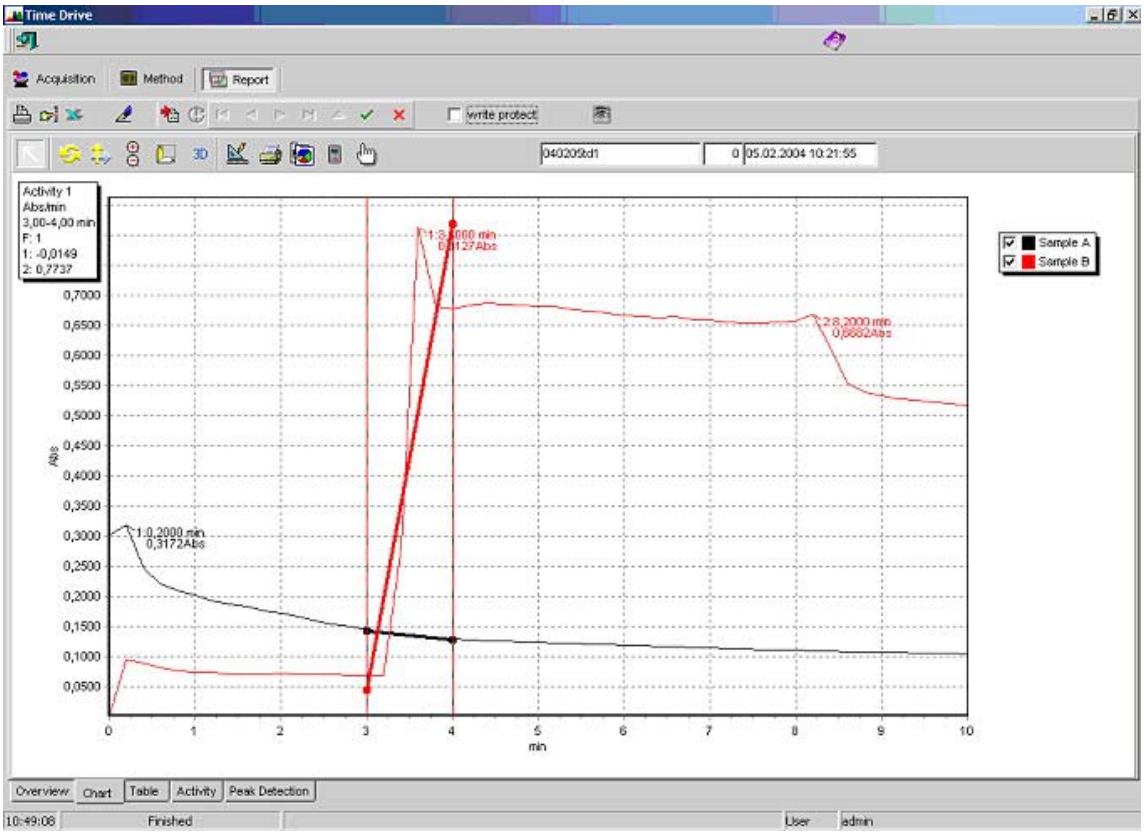
Click on the *Select Report* icon and a dialogue window appears, which allows selection of a view by date, method, user or name:



The appropriate checkboxes must be checked and, where applicable, either a date or name selected. Clicking on *OK* will cause only those reports which satisfy all selected criteria to be shown in the list of available reports.

2.4.3.3.5. The "Chart" Report Screen

Clicking on the "Chart" tab will open a new screen containing the curve in a form which can be edited:



To edit in cursor mode, uncheck the "write protect" checkbox first.

Navigation arrows are available to move between the various reports contained in the list without the need to return to the *Overview* screen.

The name of the currently displayed curve set including the revision is shown in the box display immediately above the curve display.

In *Chart* mode a range of new functions is available to the user for manipulating the presentation and properties of the current curve.

2.4.3.3.6. "Chart" Report Screen Functions

A graphics toolbar is available within the *Chart report screen*:

The use of the icons in the graphics toolbar allow direct manual manipulation of the currently displayed chart. The function of the individual icons is described briefly below:

Shows position of values on X- and Y-axis and allows to manually pick peaks and to add, edit or delete comments.

Opens the calculation dialogue window.

Exports a curve to the *Windows clipboard* for further processing.

Prints the curve as a single sheet report. Formatting of the report is described in a separate section of this document dealing with curve format.

Opens the edit dialogue for formatting functions. See the separate section of this document dealing with curve format for more details.

Converts chart format to a 3D display. The icon functions as a toggle switch between a 2D and 3D display.

Click on this icon to control the depth of the 3D display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Double function icon allowing zooming of the complete curve.

Click on this icon to move the complete curve display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Click on this icon to rotate the complete curve display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Clicking on this icon will return the function of the mouse cursor to normal thus allowing use of the normal zooming functions etc. in 3D displays.

2.4.3.4. Calculations in Time Drive

The calculation modes for curves and activities are generally embedded in the method and are described above and in detail in the Calculation section.

Recalculation after, for example, changing a *Peak Detection* parameter is possible at any time by clicking on the Calculator icon followed by selection of the parameter within the dialogue window.

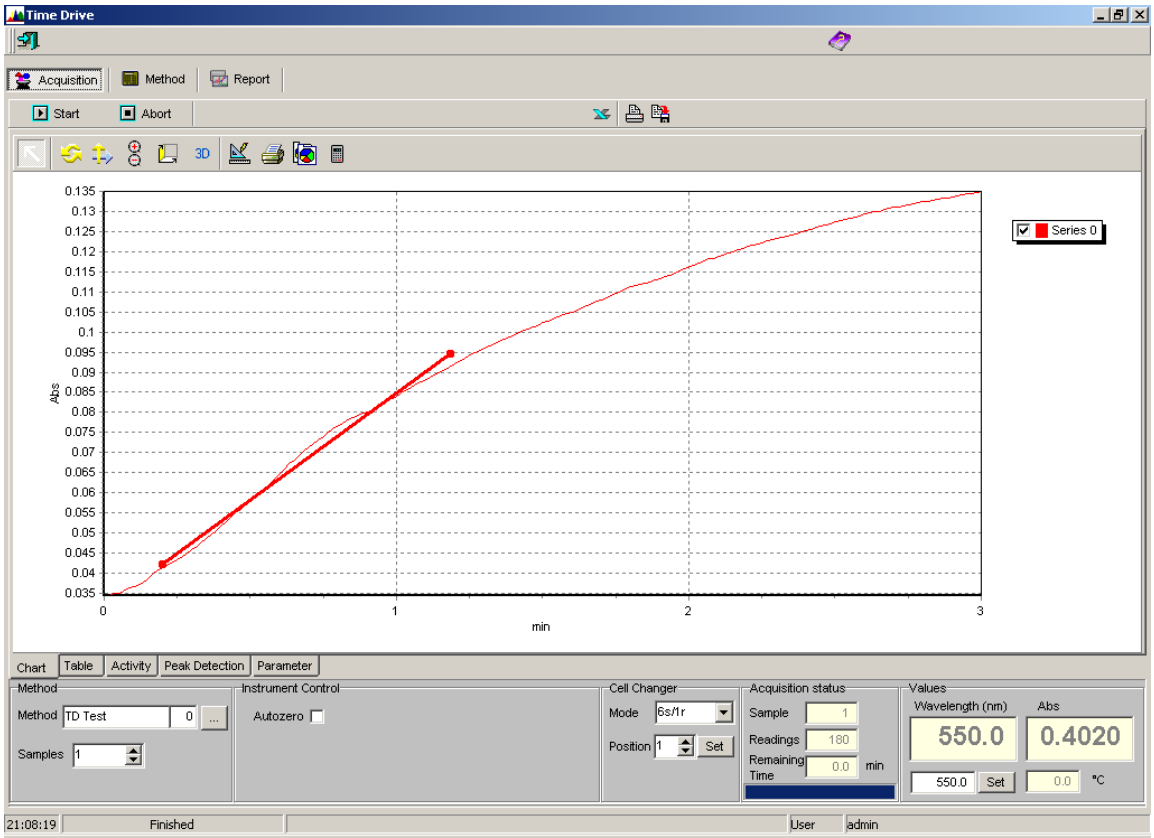
2.4.3.5. Time Drive Measurement Example

Measurement of a sample.

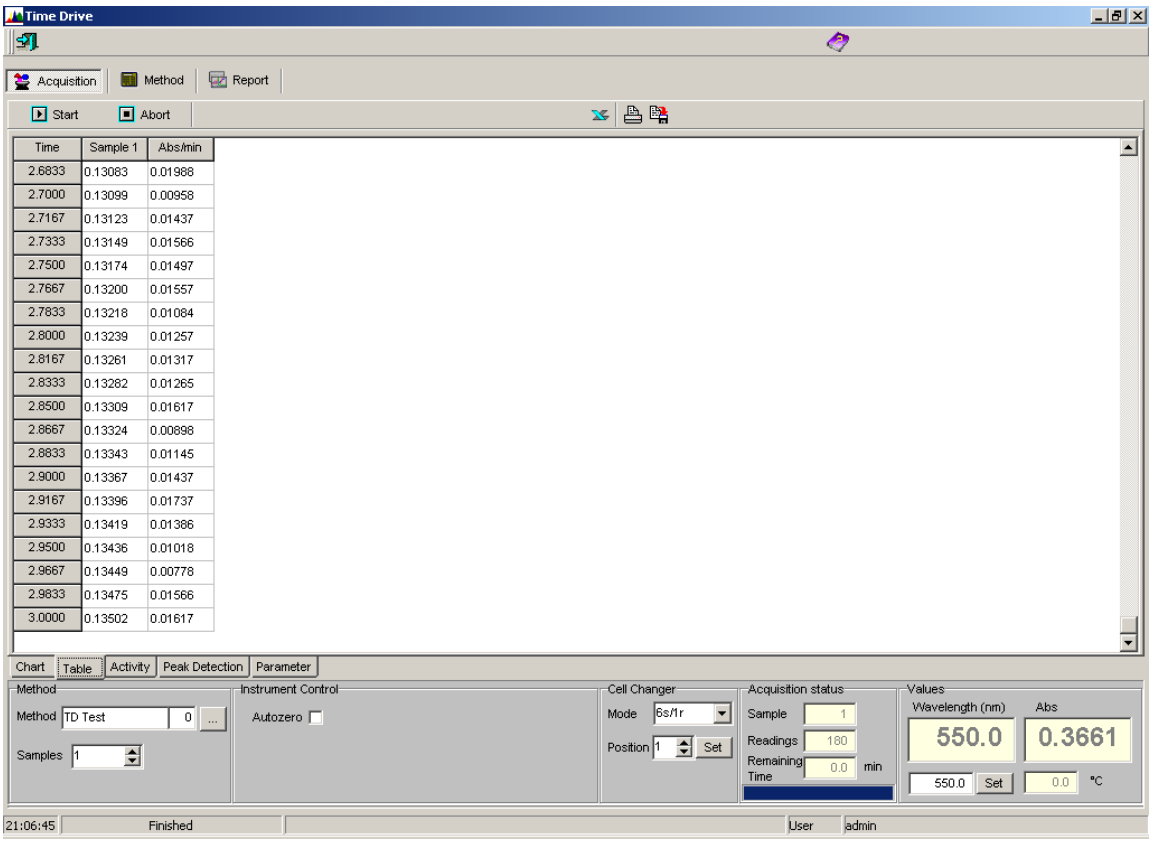
Select the method to be used and set the number of samples to 1.

Start the measurement by pressing the *Start* button and you will be prompted to insert the sample and click on *OK* to start the measurement. Insert the sample in the correct position and click on *OK*. The unit will now start to measure. The final windows will look like this:

The curve display is plotted during the acquisition and can be used to monitor the progress of the measurement. If the auto-calculation box has been checked, the regression line for the *Activity* calculation will be drawn immediately upon completion of the run.

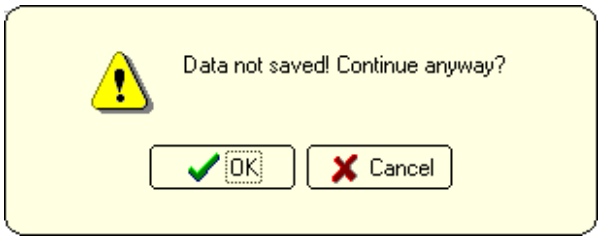


Various tab functions in the acquisition screen allow quick overviews of the results in table format (as shown below), activity etc.



Note: *If you have programmed more than one sample you will be prompted for the next sample after each sample has been measured. The final appearance of the screen remains unchanged.*

If you repeat the measurement you will always measure the selected number of samples (1 in our example) until you change the *Samples* parameter. The system will prompt if the previously run sample data has not been saved before starting a new run:



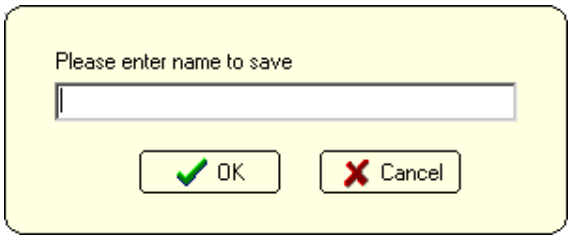
Click on *OK* to start the next acquisition run or on *Cancel* to return to the original data set.

Printing

Click on the *Print* icon to obtain a preview of the printed report, which will always contain all measurements. If the result is acceptable the report can be printed by clicking on the *Print* icon on the preview page.

Saving

Click on the *Save* icon and the system will prompt for a file name:



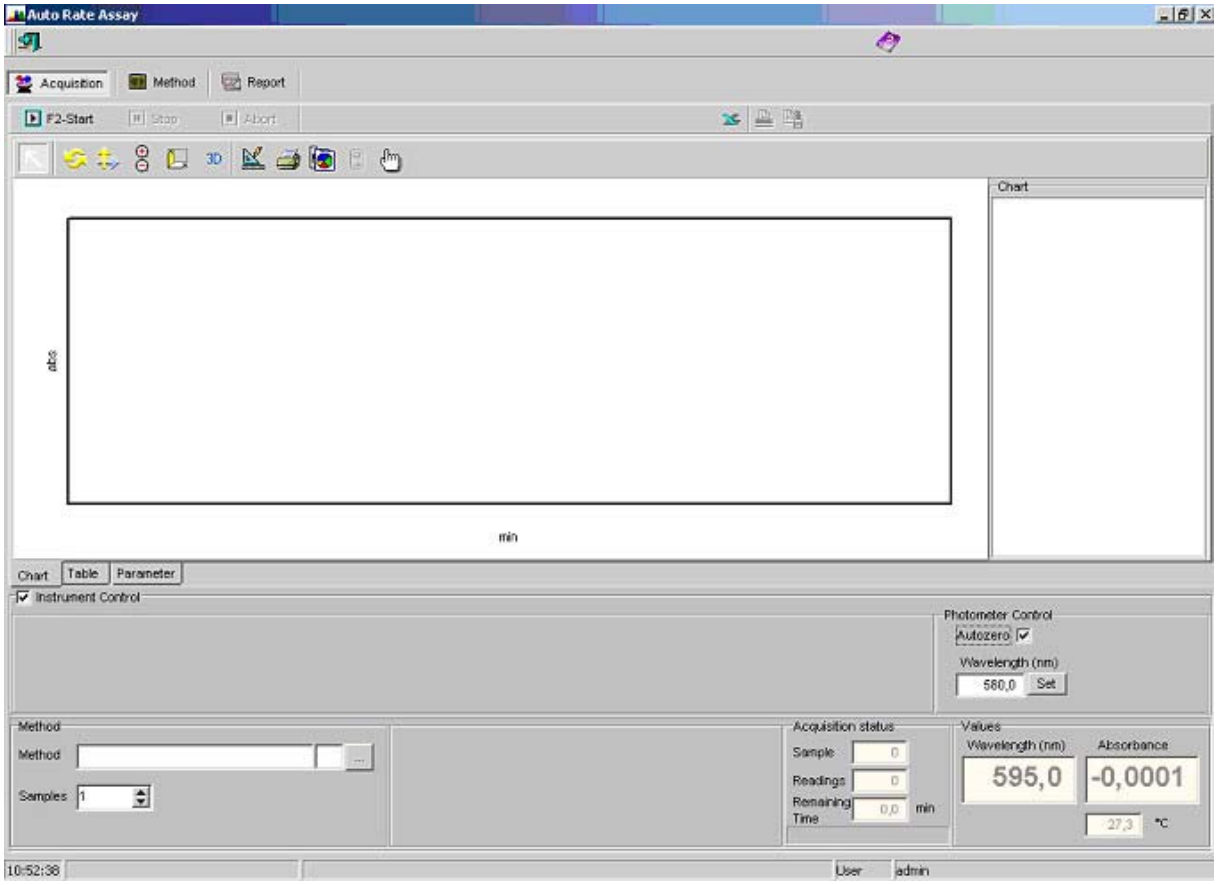
Enter the file name and click on *OK*.

2.4.4. Auto Rate Assay

The Autorate Assay mode is only possible in conjunction with an automatic cell changer. Operation is basically identical with that of Time Drive.

2.4.4.1. The Acquisition Screen in Autorate Assay

Select **"Autorate Assay"** from the main menu to obtain the following display:



This is the acquisition window from which all measurements are started. In this window the following parameters must be selected before starting a measurement:

- Method to be used for the acquisition. The method contains all parameters necessary for the execution of the measurement.
- Numbers of samples to be measured.
- *Autozero* at start of measurement.

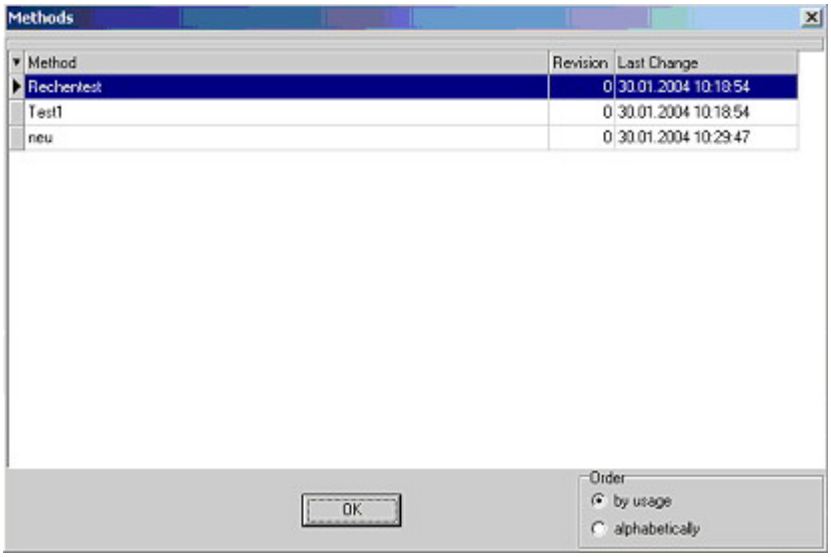
2.4.4.1.1. Run parameters

The run parameters are entered in the “Method” panel and in the “Photometer control” panel:

Samples Defines the number of samples to be analysed.

Autozero Defines whether an autozero should be executed before starting a measurement.

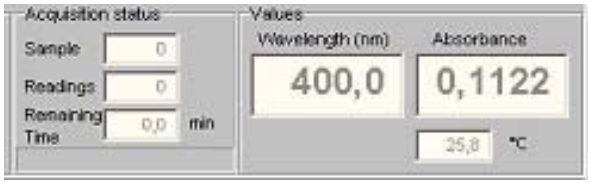
Method The method box contains the name of the method and, directly adjacent, the actual revision number of that method. The method is selected from a separate window which is opened by clicking on the button adjacent to the revision box:



This window contains a list of all available methods including all revisions of the method and the date of last modification. Selection is made by highlighting the required line and then clicking on *OK*.
The order of Methods may be displayed by usage or alphabetically.

Wavelength A certain wavelength may be chosen manually and set immediately in order to allow rapid monitoring of the unit.

2.4.4.1.2. System Status

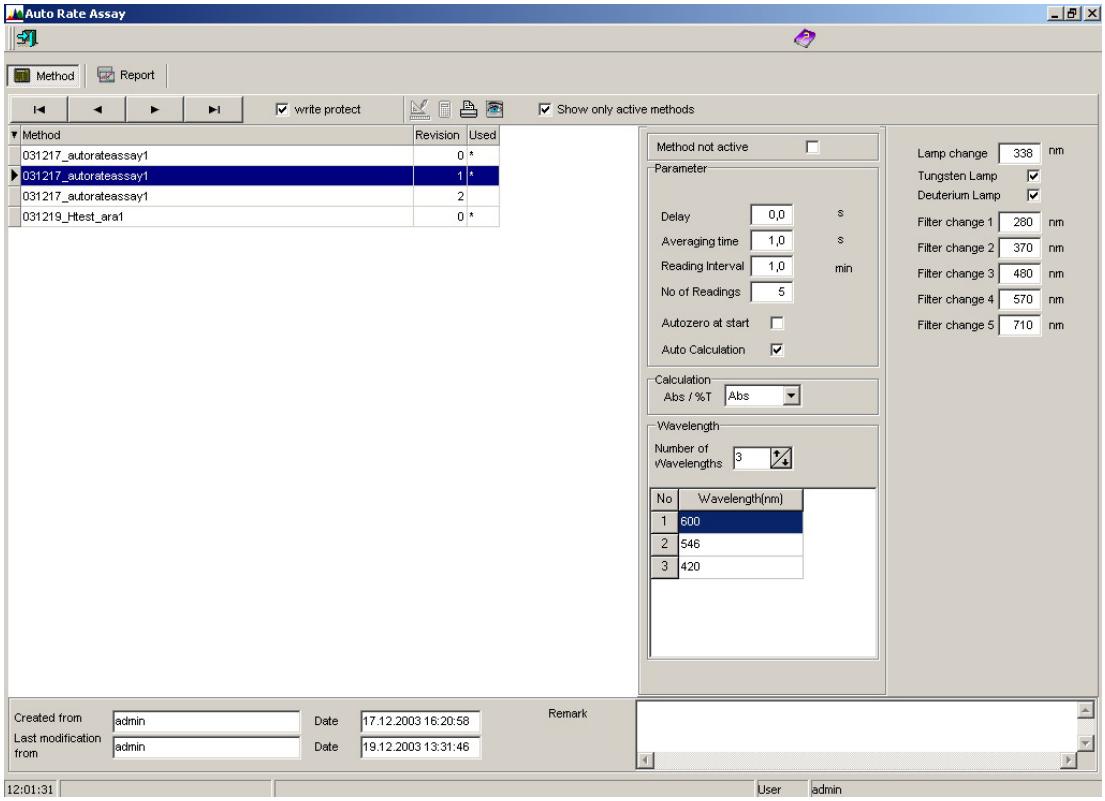


The lower right section of the display contains the actual status of the system and displays the following parameters:

- Current sample being measured.
- No. of Readings
- Remaining Time (also as progress bar)
- Actual wavelength.
- Actual absorbance value.
- Temperature (where applicable).

2.4.4.2. The Method in Autorate Assay

Click on the *Method* button in the upper left corner to open the *Method* window:



The left-hand window contains a list of all existing methods including revisions and an indication of whether they have been used already or not.

Caution: *If measurements have been used, the method will be locked and can no longer be changed. However, they can be used for later measurements or modified with revision control. Such methods are indicated by a " * " in the " used " column list.*

A new method can be created from within the method section by using the '+' button. In order to do this it is first necessary to uncheck the write-protect checkbox.

The system will first prompt for name under which the new method will be saved. Once this has been defined all other parameters can then be entered.

2.4.4.2.1. Acquisition parameters

Delay time The instrument will wait for the selected delay time after the MEASURE key is pressed to start the actual measurement.

Averaging time Defines the time the instrument uses to collect data for calculation of a mean value for one reading. A long averaging time is useful to reduce noise when measuring at high absorbance values.

Measure time Defines the actual duration of the measurement in minutes.

Sampling rate Defines the number of data points per minute for the measurement.

Autozero at start Defines whether an autozero is to be executed beforeeach sample run.

Auto Calculation If checked, the calculation for peak detection, smoothing etc. starts automatically after acquisition using the defined parameters.

Calculation mode Calculation and curve portrayal can be in either *Absorbance* or *Transmission* units.

Wavelength mode Defines the amount and the wavelengths to be used during measurement.

2.4.4.2.2. Common Parameters

The right-hand panel contains common parameters, which are required for every system and user method. They will be stored and recalled along with all other parameters.

Lamp change This parameter defines the lamp change wavelength. The deuterium lamp is used for all wavelengths below the lamp change wavelength. The tungsten halogen lamp is used for all wavelengths above the lamp change wavelength.

Tungsten lamp When checked, the tungsten lamp will be switched on and used according to the setting for the lamp change.

Deuterium lamp When checked, the deuterium lamp will be switched on and used according to the setting for the lamp change.

Filter change (1-5) This parameter defines the wavelength used to switch the filter.

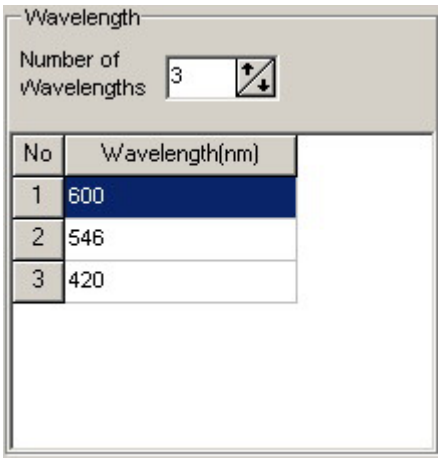
Bandwidth Selects the spectral bandwidth of the spectrophotometer.

Cell changer Defines the operating mode of the cell changer (if fitted).

2.4.4.2.3. Calculation

The calculation selection permits definition of the mode of calculation to be used. The user can select between either absorbance or transmission.

2.4.4.2.4. Wavelength



A maximum of six different wavelengths may be chosen. The λ of the wavelengths can be defined in the rows below.

2.4.4.2.5. Curve Parameters in the Auto Rate Assay Method

Opens an edit dialogue for defining curve parameters and related formatting.

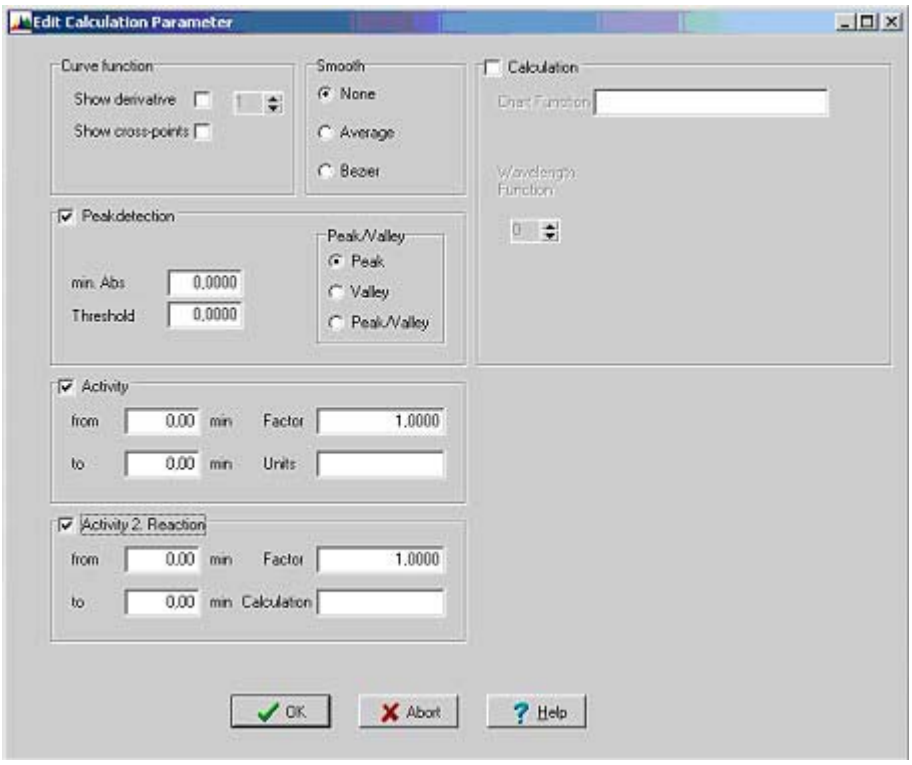
In *Auto Rate Assay* the curve parameters can be linked to a method and then define the appearance and properties of the curve such as colours, overlay format, scaling etc.

Functions defined here will be included and stored with the method and thus used for any acquisition executed utilising that method.

Formatting options using this function are described in a separate section in this document.

2.4.4.2.6. Calculation Parameters in the Auto Rate Assay Method

Click on this icon to open the calculation dialogue window for the method:

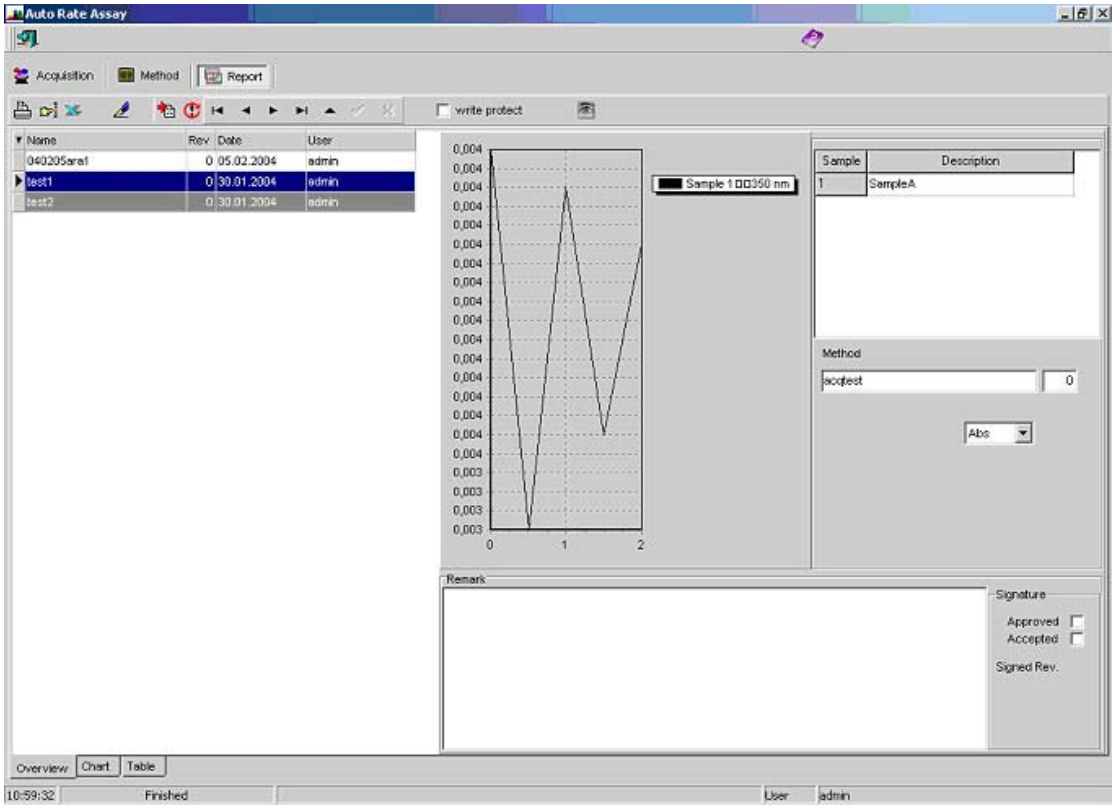


The calculation functions shown in the dialogue above are described in more detail in the section on Calculation within this document. Functions defined above will be included and stored with the method and thus used for any acquisition executed utilising that method.

2.4.4.3. The Report Screens in Autorate Assay

2.4.4.3.1. The "Overview" Report Screen

Click on the *Report* button in the upper left corner to open the *Report* window:



The display obtained is the "Overview" screen, clicking on the "Chart" tab will display the chart as the main item which can be manipulated or edited as required.

The tabs for *Activity* and *Peak Detection* show a display in table form for the respective parameters

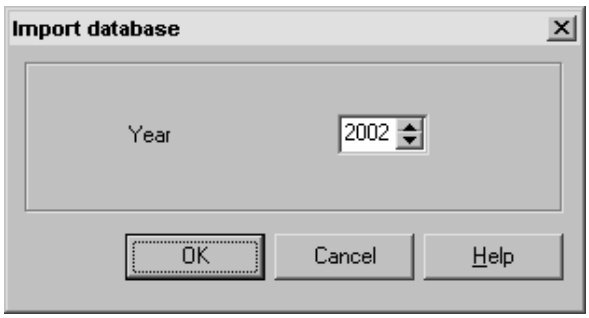
The left-hand window contains a list of all available reports, the right-hand window contains the results in the upper section and the main parameters for the measurement in the lower part. Each report can be viewed by scrolling through the left-hand list.

2.4.4.3.2. Printing

Click on the *Print* icon to obtain a print preview of the selected report, which will always contain all measurements. The report can be printed by clicking on the *Print* icon on the preview page.

2.4.4.3.3. Importing a report from the database

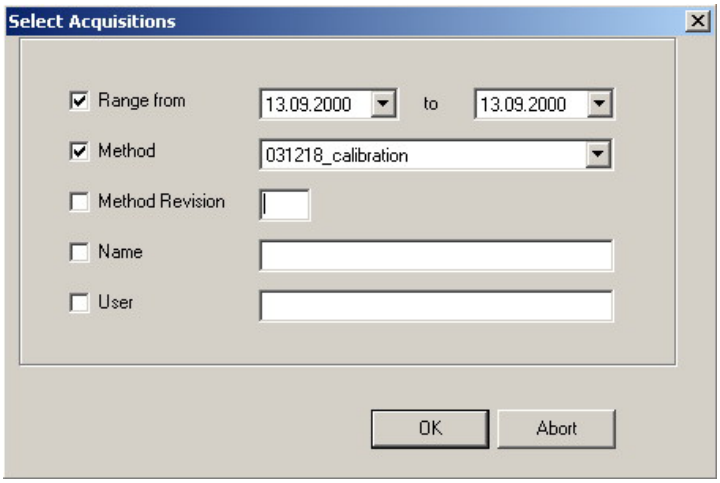
Click on the import icon to access earlier reports in the archived database. A dialogue window for selection of the database will be opened:



2.4.4.3.4. Filtering the report list

The report list in the left window will become very long with time and it may be necessary to filter the list so that only files of interest are shown to a user. This is carried out using the *Select Report* icon.

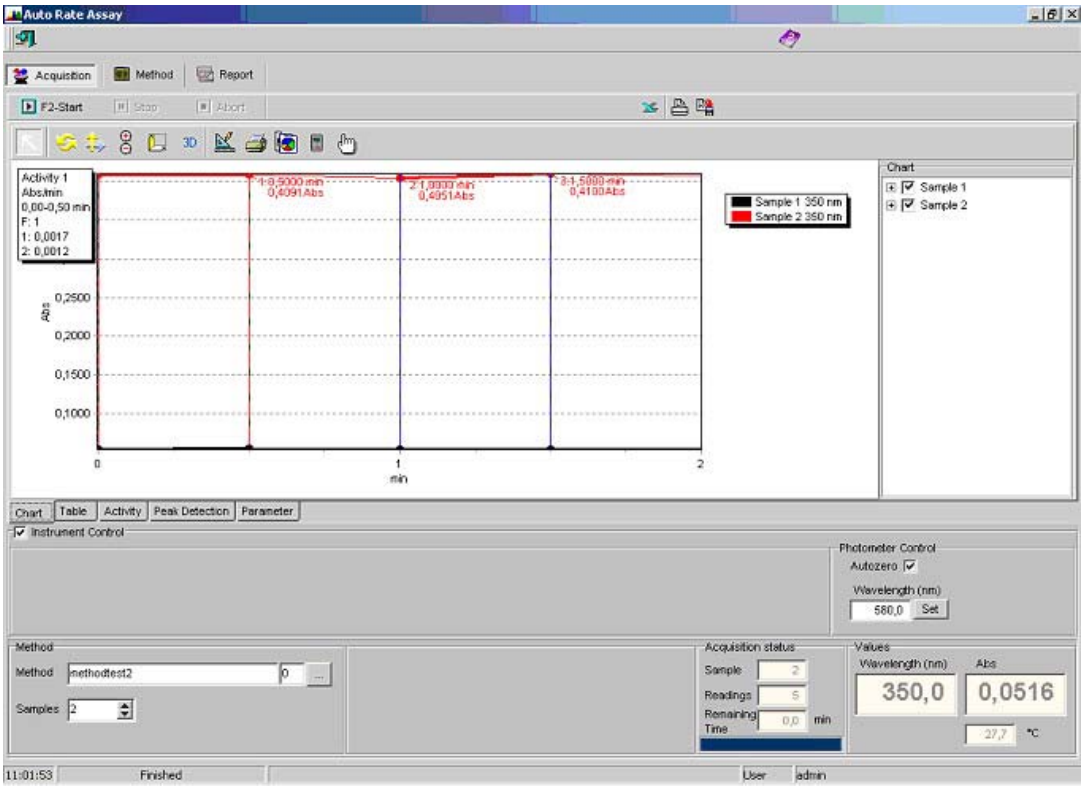
Click on the *Select Report* icon and a dialogue window appears, which allows selection of a view by date, method, user or name:



The appropriate checkboxes must be checked and, where applicable, either a date or name selected. Clicking on *OK* will show only those reports which match with selected criteria shown in the list of available reports.

2.4.4.3.5. The "Chart" Report Screen

Clicking on the "Chart" tab will open a new screen containing the curve in a form which can be edited:



Navigation arrows are available to move between the various reports contained in the list without the need to return to the *Overview* screen.

The name of the currently displayed curve set including the revision is shown in the box display immediately above the curve display.

In *Chart* mode a range of new functions is available to the user for manipulating the presentation and properties of the current curve.

2.4.4.3.6. "Chart" Report Screen Functions

A graphics toolbar is available within the *Chart report screen*:

The use of the icons in the graphics toolbar allow direct manual manipulation of the currently displayed chart. The function of the individual icons is described briefly below:

Shows position of values on X- and Y-axis and allows to manually pick peaks and to add, edit or delete comments.

Opens the calculation dialogue window.

Exports a curve to the *Windows clipboard* for further processing.

Prints the curve as a single sheet report. Formatting of the report is described in a separate section of this document dealing with curve format.

Opens the edit dialogue for formatting functions. See the separate section of this document dealing with curve format for more details.

Converts chart format to a 3D display. The icon functions as a toggle switch between a 2D and 3D display.

Click on this icon to control the depth of the 3D display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Double function icon allowing zooming of the complete curve.

Click on this icon to move the complete curve display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Click on this icon to rotate the complete curve display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Clicking on this icon will return the function of the mouse cursor to normal thus allowing use of the normal zooming functions etc. in 3D displays.

2.4.4.4. Calculations in Autorate Assay

The calculation modes for curves and activities are generally embedded in the method and are described above and in detail in the Calculation section.

Recalculation after, for example, changing a *Peak Detection* parameter is possible at any time by clicking on the *Calculator* icon followed by selection of the parameter within the dialogue window.

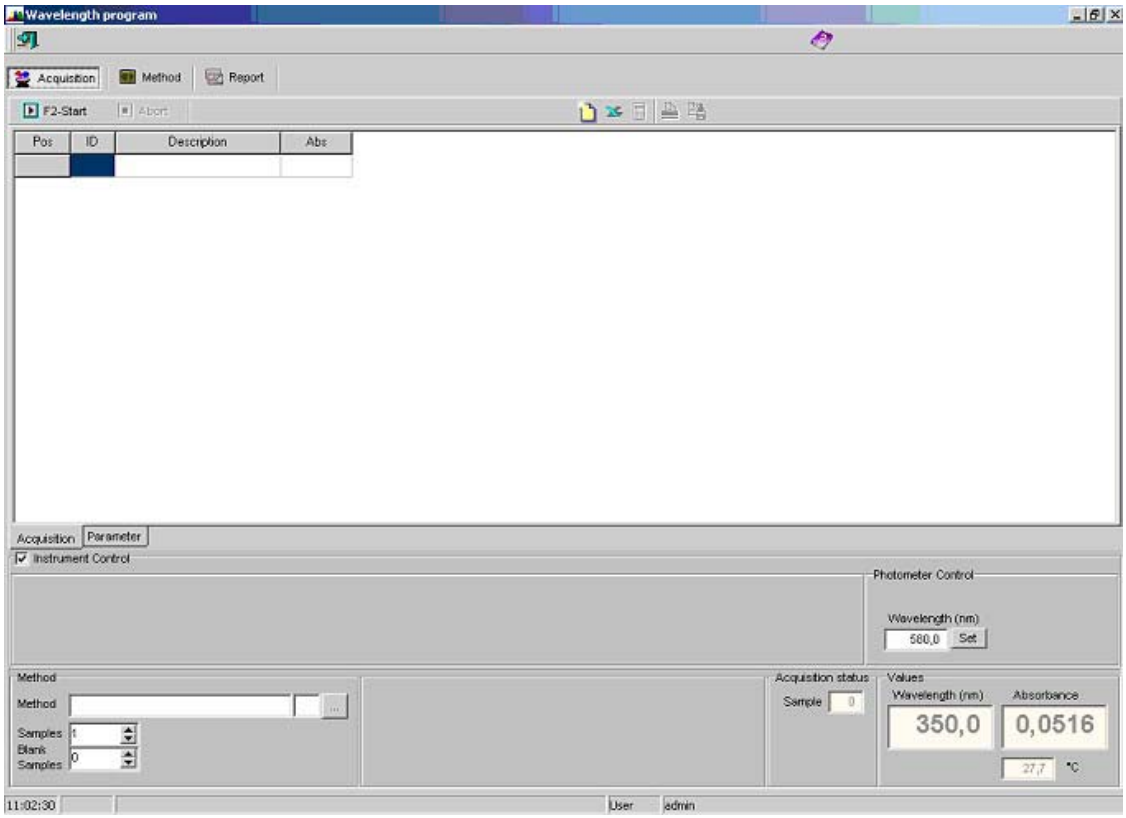
2.4.5. Wavelength Program

Wavelength Program mode permits measurements at different wavelengths and also calculations such as wavelength ratios to be made automatically for a set of samples.

The first samples measured can be defined as *Blanks* and the values of these samples will be averaged and then subtracted from each wavelength measurement of that particular sample.

2.4.5.1. The Acquisition Screen in Wavelength Program

Select **"Wavelength Program"** from the main menu to obtain the following display:



This is the acquisition window from which all measurements are started. In this window the following parameters must be selected before starting a measurement:

- Method to be used for the acquisition. The method contains all parameters necessary for the execution of the measurement.
- Numbers of samples to be measured.
- Number of blank samples, measured as the first samples.
- *Autozero* at start of measurement.

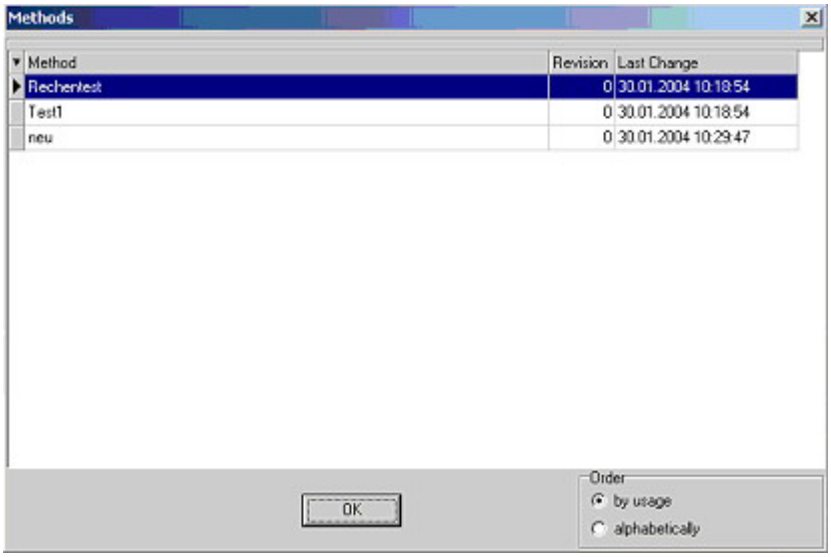
2.4.5.1.1. Run parameters

The run parameters are entered in the “Method” panel and in the “Photometer control” panel:

Samples Defines the number of samples to be analysed.

Blank Samples Defines the number of blank samples to be measured, blank samples are always expected at the start of a run. The value of the measured blank is subtracted from the actual measured value of the sample prior to calculation of concentration etc. If more than one blank is defined then the system calculates the average blank value for the blanks and then subtracts this from the actual measured sample values.

Method The method box contains the name of the method and, directly adjacent, the actual revision number of that method. The method is selected from a separate window which is opened by clicking on the button adjacent to the revision box:



This window contains a list of all available methods including all revisions of the method and the date of last modification. Selection is made by highlighting the required line and then clicking on *OK*.
The order of Methods may be displayed by usage or alphabetically.

Wavelength A certain wavelength may be chosen manually and set immediately in order to allow rapid monitoring of the unit.

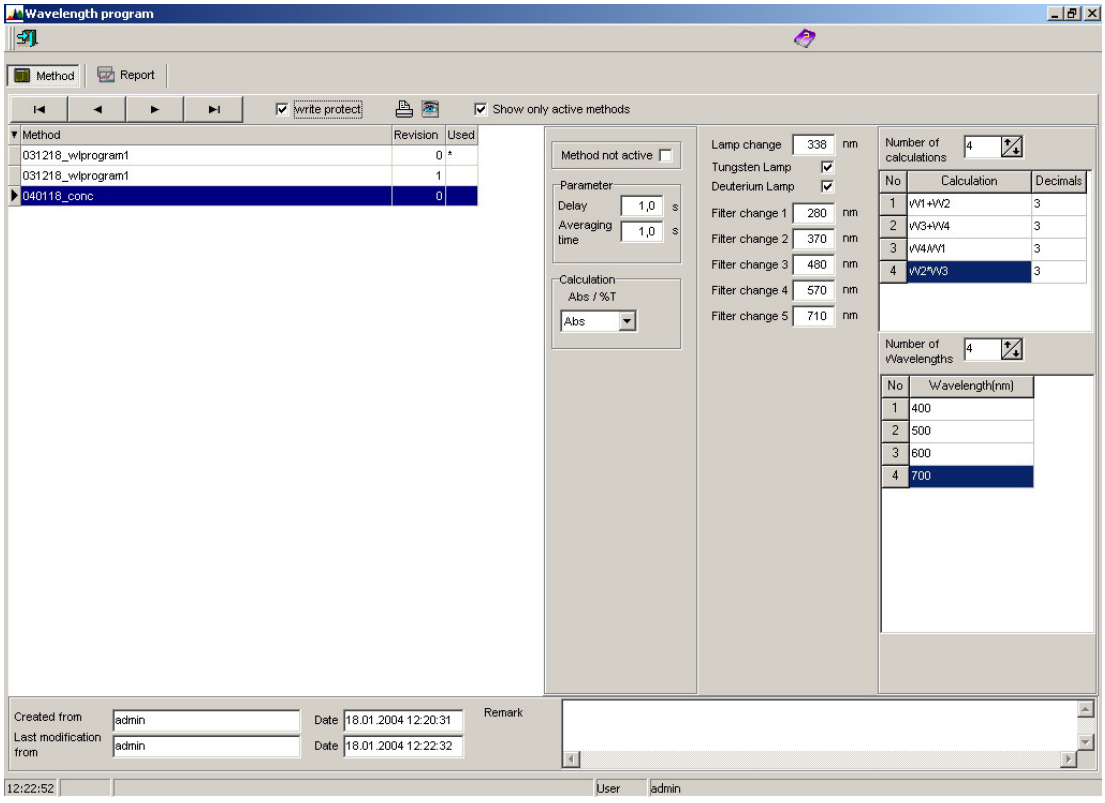
2.4.5.1.2. System Status

The lower right section of the display contains the actual status of the system and displays the following parameters:

- Current sample being measured.
- Actual wavelength.
- Actual absorbance value.
- Temperature (where applicable).

2.4.5.2. The Method in Wavelength Program

Click on the *Method* button in the upper left corner to open the *Method* window:



The left-hand window contains a list of all existing methods including revisions and an indication of whether they have been used already or not.

Caution: *If measurements have been used, the method will be locked and can no longer be changed. However, they can be used for later measurements or modified with revision control. Such methods are indicated by a " * " in the " used " column list.*

A new method can be created from within the method section by using the '+' button. In order to do this it is necessary to uncheck the write-protect checkbox.

The system will first prompt for name under which the new method will be saved. Once this has been defined all other parameters can then be entered.

2.4.5.2.1. Acquisition parameters

Delay time The instrument will wait for the selected delay time after the MEASURE key is pressed to start the actual measurement.

Averaging time Defines the time the instrument uses to collect data for calculation of a mean value for one reading. A long averaging time is useful to reduce noise when measuring at high absorbance values.

2.4.5.2.2. Common parameters

The right-hand panel contains common and calculations parameters, which are required for every system and user method. They will be stored and recalled along with all other parameters:

Lamp change This parameter defines the lamp change wavelength. The deuterium lamp is used for all wavelengths below the lamp change wavelength. The tungsten halogen lamp is used for all wavelengths above the lamp change wavelength.

Tungsten lamp When checked, the tungsten lamp will be switched on and used according to the setting for the lamp change.

Deuterium lamp When checked, the deuterium lamp will be switched on and used according to the setting for the lamp change.

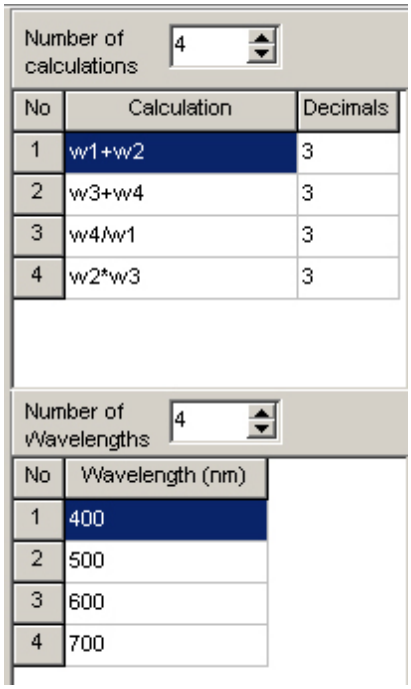
Filter change (1-5) This parameter defines the wavelength used to switch the filter.

Bandwidth Selects the spectral bandwidth of the spectrophotometer.

Cell changer Defines the operating mode of the cell changer (if fitted).

2.4.5.2.3. Wavelength Program calculations

The right section of the method screen allows definition of the wavelengths to be used and also the calculation modes:



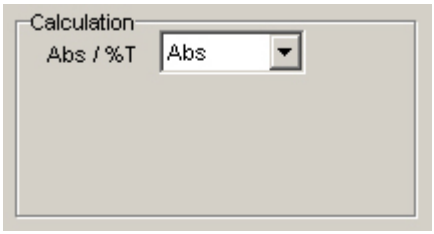
The required number of both calculations and wavelengths to be used must first be defined using the two spin boxes at the top of each entry window. This definition will open the appropriate number of lines where the actual values can be entered directly:

Calculation: Wavelengths are defined for calculation purposes as W(n) or w(n) respectively, where (n) corresponds to actual number for a given wavelength as shown in the lower window. In the example above the following calculations will be performed:

1.	Wavelength number 1, e.g. at 400 nm is added to	Wavelength 2.
2.	Wavelength number 3, e.g. at 600 nm, is added to	Wavelength 4
3.	Wavelength number 4, e.g. at 700 nm is divided by	Wavelength 1
4.	Wavelength number 2, e.g. at 500 nm, is multiplied by	Wavelength 3

Decimals: The number of decimal places to be used for the calculation can also be defined. This number should generally be consistent with the actual measured result, e.g. by measurements to 4 decimal places, selection of a much higher number for the calculation result will not increase the accuracy of a measurement or result and could produce rounding errors.

2.4.5.2.4. Calculation



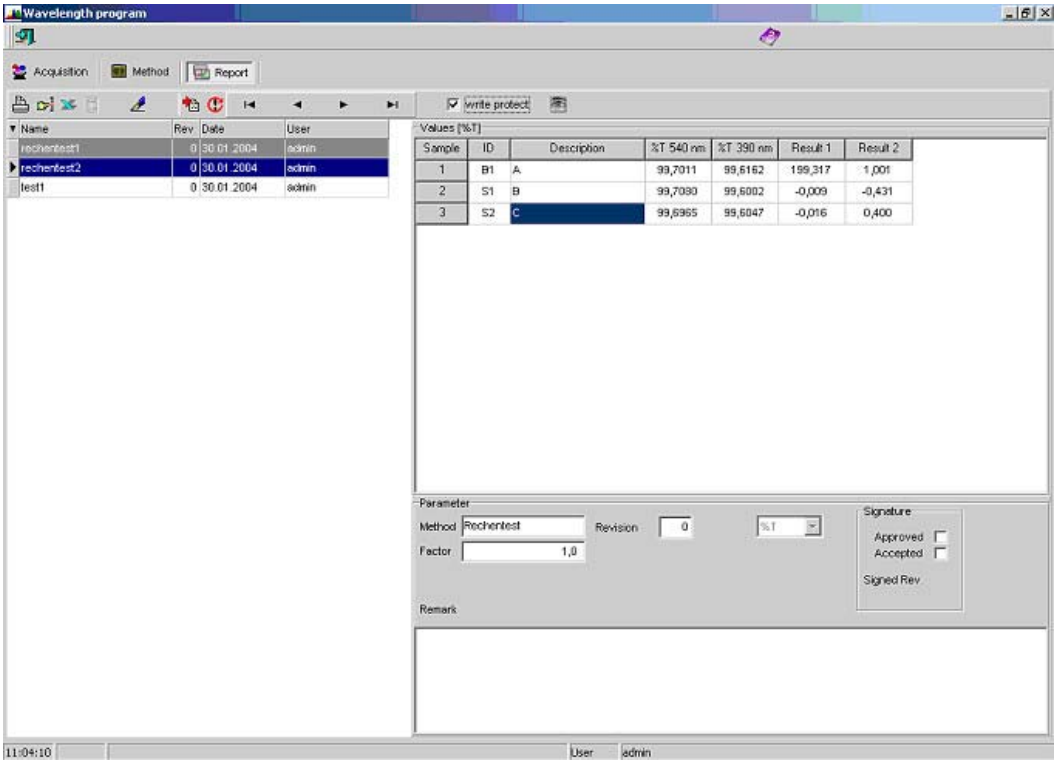
The calculation selection permits definition of the mode of calculation to be used, the user can select between either absorbance or transmission.

2.4.5.2.5. Audit Trail in Wavelength Program Method

Click on the *Audit Trail* icon to view the audit trail window for a method.

2.4.5.3. The Report Screen in Wavelength Program

Click on the *Report* button in the upper left corner to open the *Report* window:



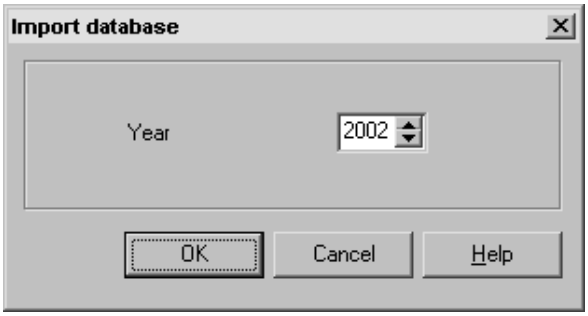
The left-hand window contains a list of all available reports, the right-hand window contains the results in the upper section and the main parameters for the measurement in the lower part. Each report can be viewed by scrolling through the left-hand list. Data can be viewed in the right-hand window by scrolling across the table using the mouse.

2.4.5.3.1. Printing

Click on the *Print* icon to obtain a print preview of the selected report, which will always contain all measurements. The report can be printed by clicking on the *Print* icon on the preview page.

2.4.5.3.2. Importing a report from the database

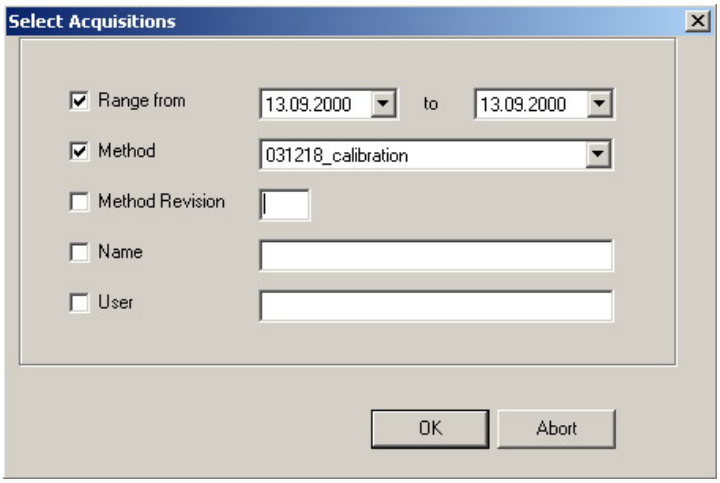
Click on the import icon to access earlier reports in the extracted database. A dialogue window for selection of the database will be opened:



2.4.5.3.3. Filtering the report list

The report list in the left window will become very long with time and it may be necessary to filter the list, so that only files of interest are shown to a user, using the *Select Report* icon:

Click on the *Select Report* icon and a dialogue window appears, which allows selection of a view by date, method, user or name:



The appropriate checkbox must be checked and, where applicable, either a date or name selected. Clicking on *OK* will cause only those reports which match with selected criteria shown in the list of available reports.

2.4.5.3.4. Audit Trail in Wavelength Program Report

Click on the *Audit Trail* icon to view the audit trail window for a report:

2.4.5.4. Calculations in Wavelength Program

Wavelength Program contains, alongside the basic wavelength calculations described above, two additional calculation methods for the final result determination:

- Blank
- Factor

In *Wavelength Program* the *Blank* and *Factor* calculations can be executed automatically without the need to create a calibration file:

Blank The measured values for sample blank at each wavelength is subtracted from the measured value of each measured sample at the same wavelength.

Factor The actual value obtained from the measurement is always multiplied by the factor parameter. This is accessible by clicking on the *Parameter* tab in the acquisition screen.

The actual calculation is based on the following formula at any given wavelength:

$$RW = F * (VM_{sample} - VM_{blank})$$

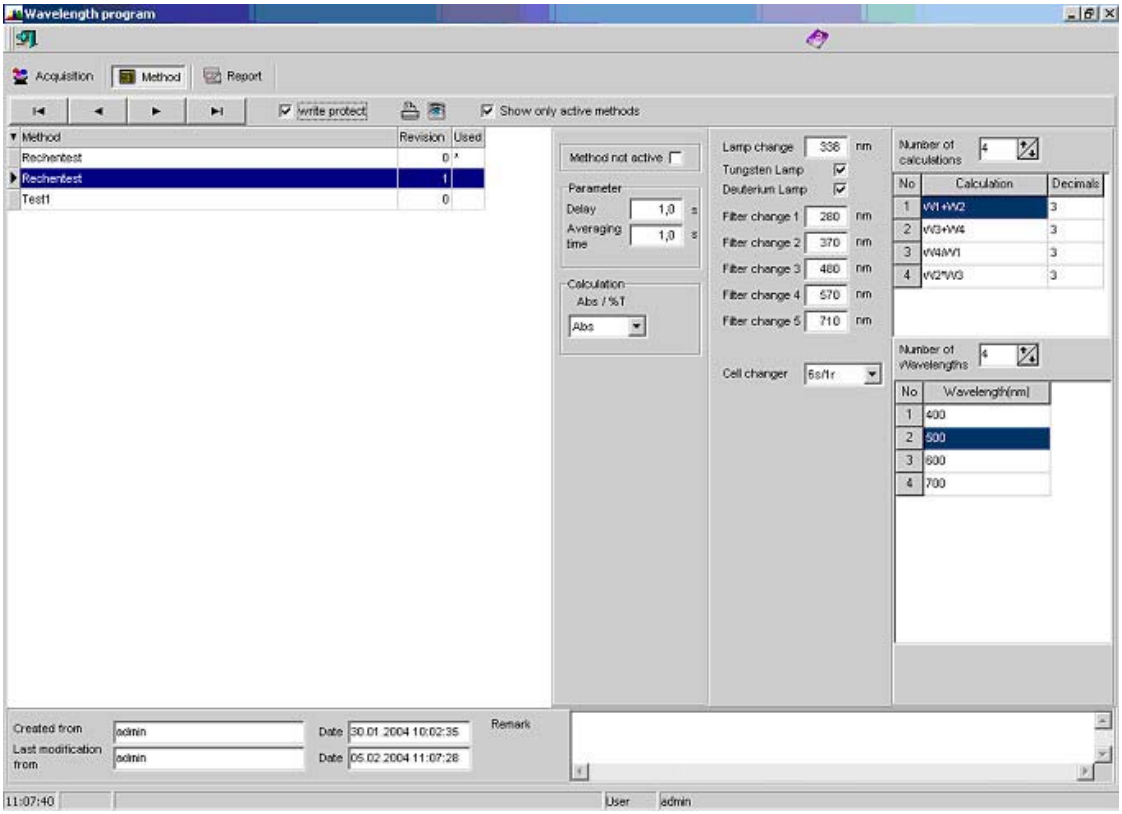
Where RW = Result for wavelength W, F = Factor and VM represents the measured values obtained for sample and blank respectively. The value RW is then used for the defined calculations for the individual wavelengths.

Recalculation after, for example, changing the factor value is possible at any time by clicking on the *Calculator* icon **before** the data has been saved..

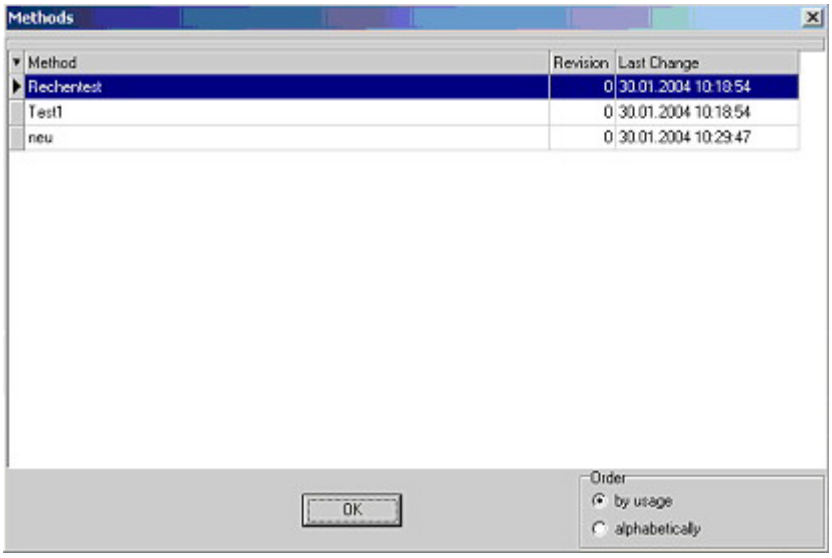
2.4.5.5. Wavelength Program Measurement Example

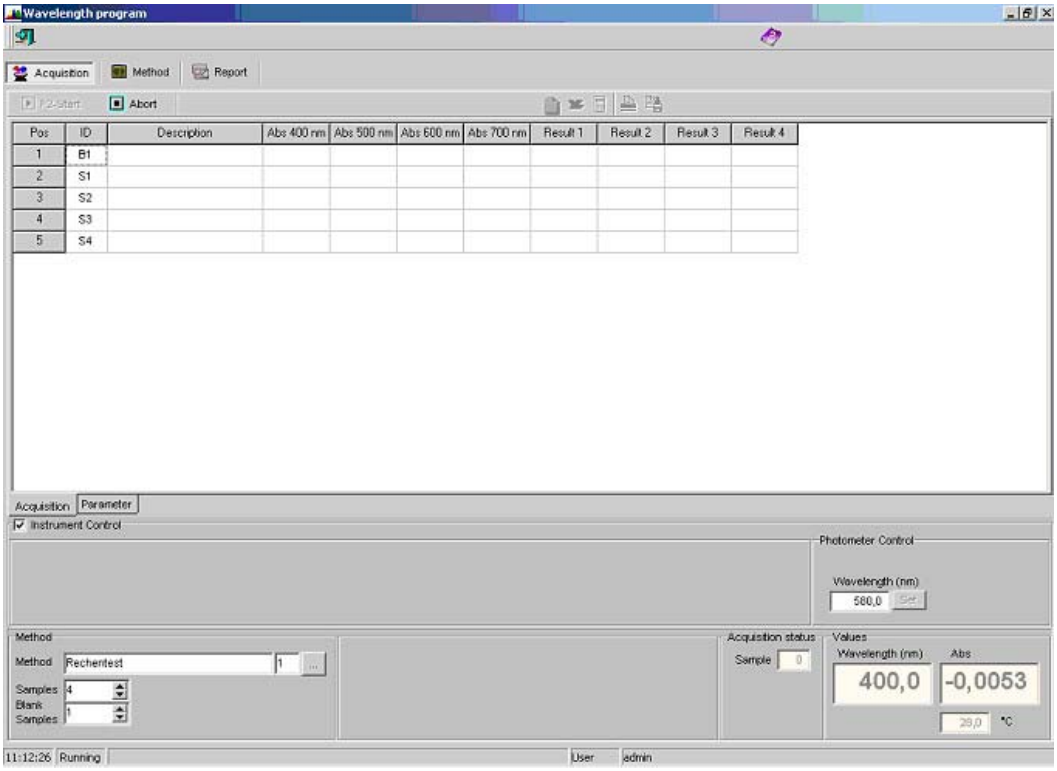
Wavelength Program measurement of 4 samples using an optional automatic 6+6 cell changer. Four wavelengths are used (400, 500, 600 and 700 nm). The first sample is a Blank.

Define the method to be used:

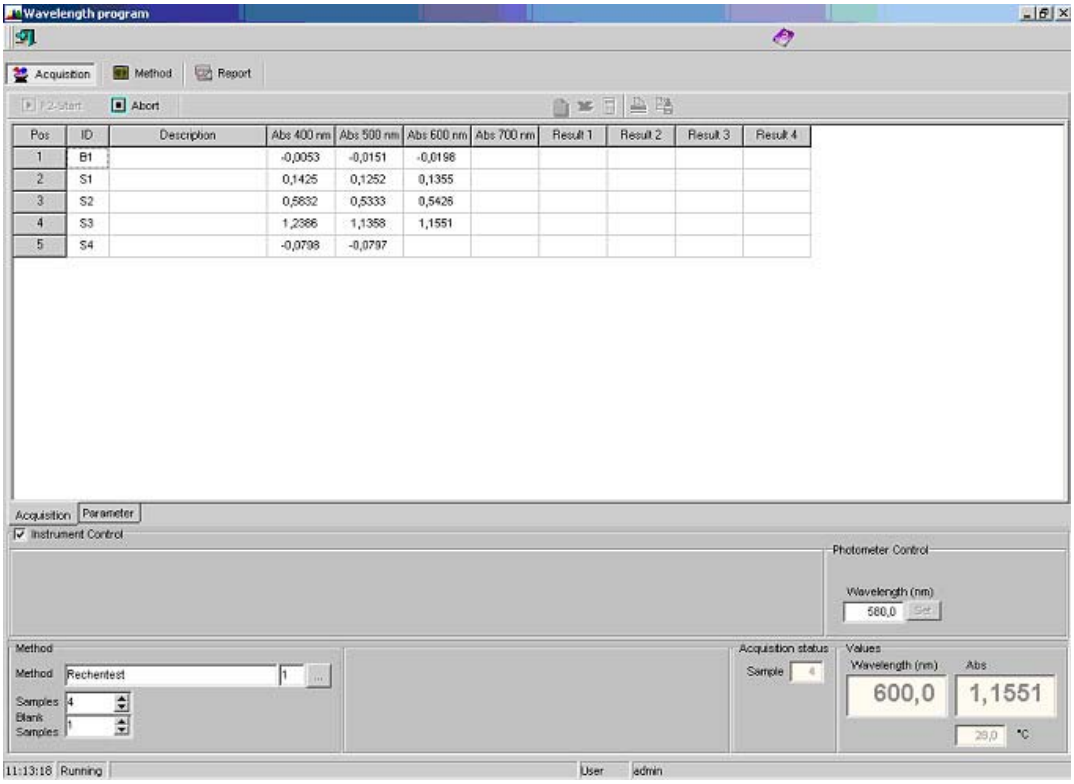


Click on the *Acquisition* tab in the upper left corner and select a method by clicking on the button next to the method window in the lower left of the screen:

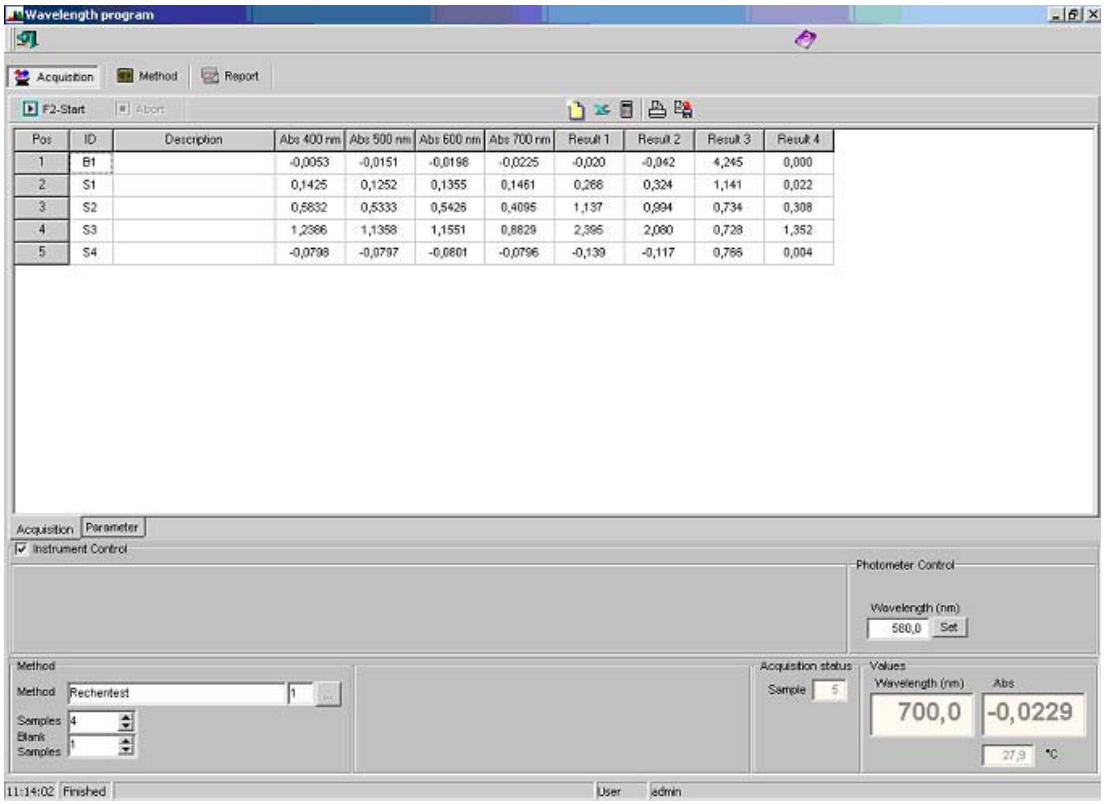




Set the number of samples to 4 and the Blank Samples to 1. Enter descriptions if required and insert the *Blank* sample in position 1 in the cell changer and the four samples in positions 2 to 5. Start the measurement by pressing the *Start* button. The measured values will be displayed during acquisition:

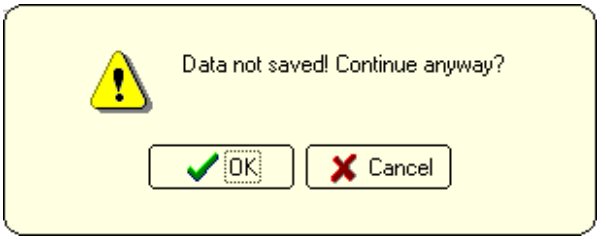


The final window will look like this:



Note: *If you are not using a cell changer, you will be prompted for the next sample after each sample has been measured. The final appearance of the screen remains unchanged.*

If you repeat the measurement you will always measure the selected number of samples (3 in our example) until you change the *Samples* parameter. The system will prompt if the previously run sample data has not been saved before starting a new run:



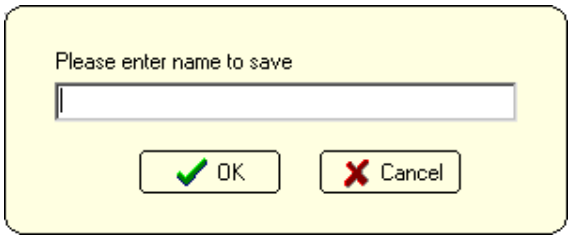
Click on *OK* to start the next acquisition run or on *Cancel* to return to the original data set.

Printing

Click on the *Print* icon to obtain a preview of the printed report, which will always contain all measurements. If the result is acceptable the report can be printed by clicking on the *Print* icon on the preview page.

Saving

Click on the *Save* icon and the system will prompt for a file name:



Enter the file name and click on *OK*.

2.5. CALCULATIONS

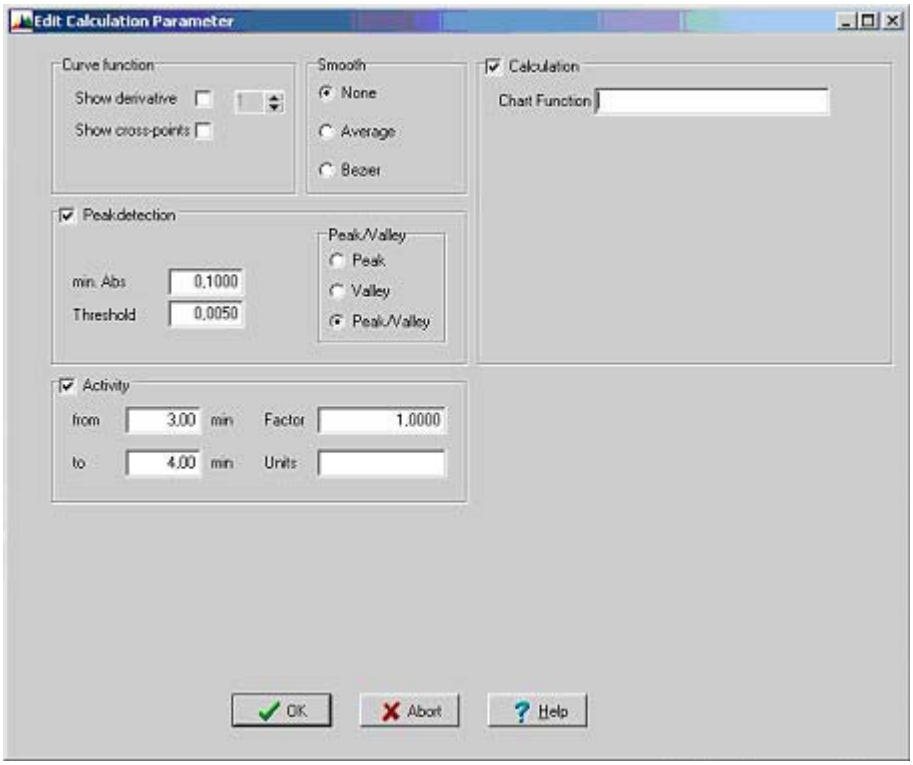
The UVS software contains various calculation possibilities depending on the selected measuring mode.. These calculations are accessible using the *Calculator* icon.

2.5.1. Curve Functions

Calculations based on charts can be executed in one of two ways:

- Post-run by clicking on the *Report* tab in the report section and then the calculator icon in order to obtain the calculation dialogue.
- Definition of the required calculations as a part of the method in which case they can be executed automatically at the end of the run.

Click on the calculator icon in either the *Method* or *Report* screen in order to obtain the calculation dialogue:



The functions available for manipulation of curve data are the following:

- Derivatives up to 4th derivative
- Cross-points
- Smoothing
- Mathematical calculations on a complete curve
- Peak detection
- Activity

2.5.1.1. Derivative

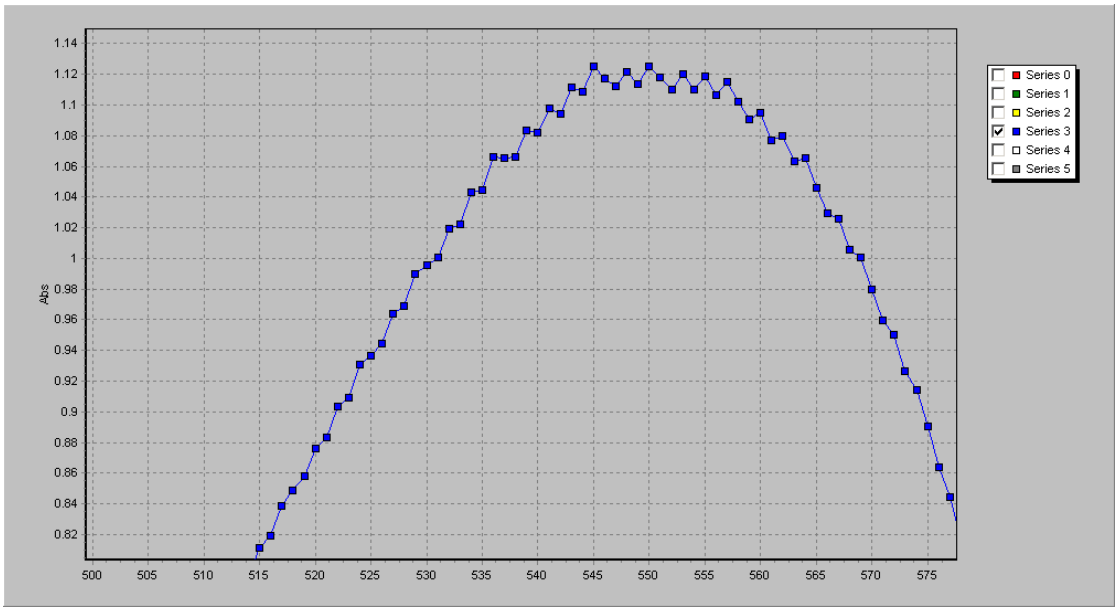
The software allows direct calculation of derivative orders 1 to 4 for *Wavelength Scan* and *Time Drive* data. A separate optimised calculation algorithm is used for each order therefore the quality of the result will be much improved if you calculate, for example, a fourth derivative directly from a loaded zero order curve.

To display a derivative click on the “Show derivative” checkbox, which will open the spinbox for selection of the required order.

Set the required derivative order in the spinbox and click on OK. The curve display will automatically change to show the new derivative curve.

2.5.1.2. Show cross-points

Selecting the *Show* cross-points parameter will display each data point collected on the curve as shown in the zoomed example below:



2.5.1.3. Smoothing

A filter can be introduced in the data acquisition in order to reduce noise. Smoothing can be selected with as an averaging or a Bezier function.

High smoothing will reduce noise, however high smoothing will also reduce the amplitude of the peaks obtained and can also result in distortion of peak shape.

Average This is a rolling average function based on 3 calculated points. Only Y values are calculated.

$$P(x) = [x_{(n-1)}+x_{(n)}+x_{(n+1)}] / 3$$

Bezier A Bezier curve is an approximation to a curve which would pass through all the control points. The method used here for defining such a curve approximation is called the Bezier-Bernstein approximation.

2.5.1.4. Calculation

The calculation function allows definition of mathematical functions which can be used to modify the curve data. “S” is used to denote the sample itself and calculations are defined simply using “S” and the appropriate factor (F) and signs:

Addition: Enter F+S

Subtraction: Enter S-F

Multiplication: Enter F*S

Division: Enter S/F

For example it is also possible to subtract an offset from each point in the curve and then double the signal level and this would be programmed as follows:

Click on the *Calculation* checkbox and then enter the required formula, in this example the formula would simply be 2*(S-0.2).

Caution *Please note that spaces are not permitted in the formula.*

2.5.1.5. Peak Detection

This calculation mode can be used with the system methods: *Wavelength Scan*, *Time Drive* and *Auto Rate Assay*.

Peak detection can be linked to a method and carried out during or after measurement. To activate peak detection select **“Peak detection”** in the calculation parameter editor window.

A peak is detected when the slope of the curve changes from positive to negative, a valley is detected when the slope changes from negative to positive.

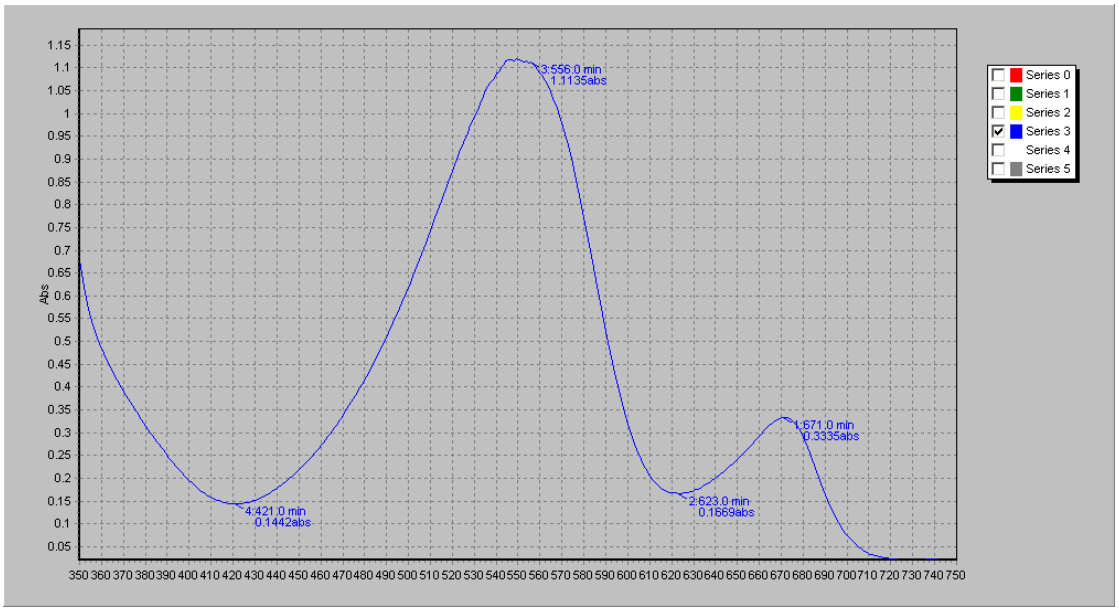
After selecting **“Peak detection”** it is possible to set the following parameters:

Min. Abs The Min. Abs. parameter defines the absolute minimum value for a peak or valley to be detected, any peak or value with an absorbance value lower than the defined value will be ignored.

Threshold The threshold is the difference in height on the Y-axis between two peaks or valleys. If the difference between valley and peak is lower than the set threshold then the peaks/valleys will not be detected.

Peak / Valley The selection defines whether the calculation is to be made for peaks only, valleys only or both peaks and valleys.

If peak detection has been selected the results can be seen both in the peak detection table and directly on the curve itself:

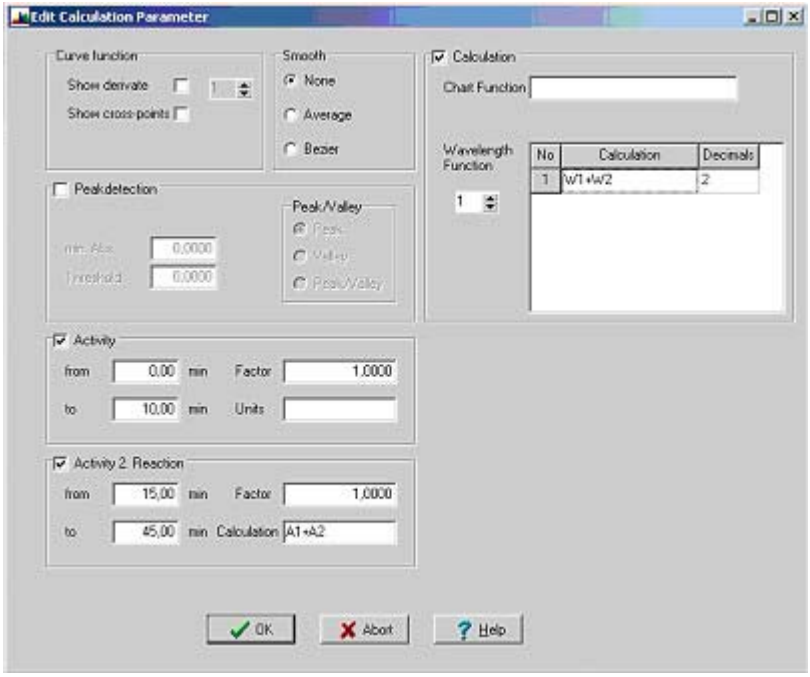


2.5.2. Activity

This calculation mode can be used in the system methods *Time Drive* and *Auto Rate Assay*. An activity of the second reaction can be used exclusively in the system method *Auto Rate Assay*. It is used to calculate the activity of reactions. Calculation of the activity is made using a linear regression model.

The calculation can be embedded in the method such that it is performed automatically at run end or it can be executed manually after acquisition.

Selection of the parameters for the *Activity* calculation is made, as above, by clicking on the *Calculator* icon in either the *Method* or *Report* screens. Click on the *Calculator* icon to obtain the appropriate dialogue box and then click on the *Activity* checkbox.



It is possible to define the section of the curve over which the calculation is to be made, a factor and the units for the *Activity* value:

It is now possible to set directly the following parameters:

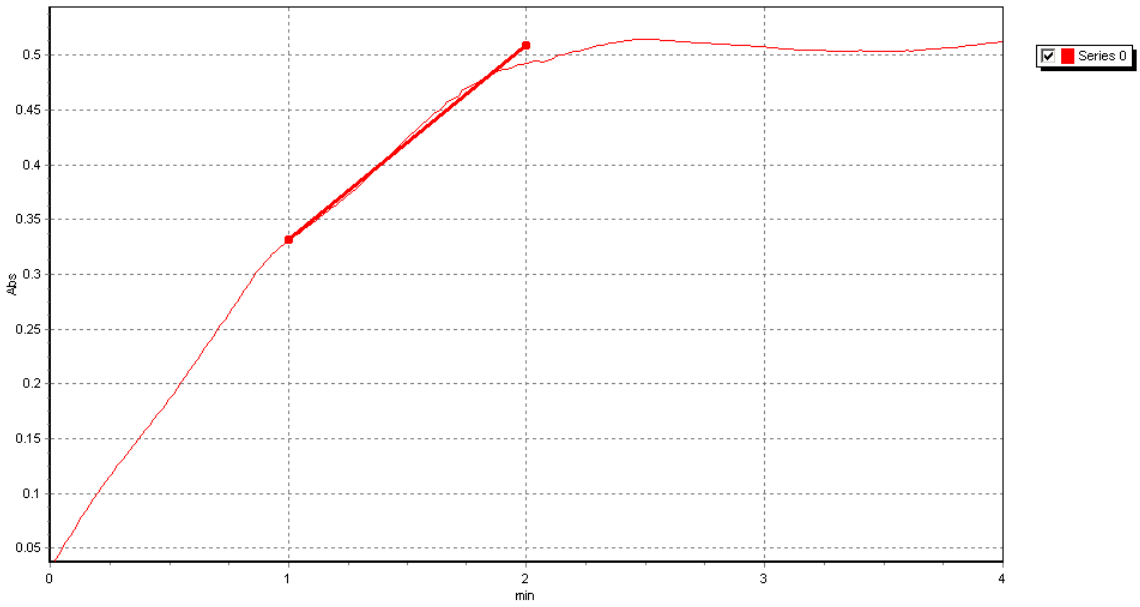
From Defines the lower starting point on the curve time-scale for the range of the *Activity* calculation.

to Defines the upper starting point on the curve time-scale for the range of the *Activity* calculation.

Factor Activity is calculated by multiplying the slope of the regression line (Absorbance change per minute) by the factor (**F**).

Units Defines the units to used for reports etc., e.g. Abs/min., µmol/min

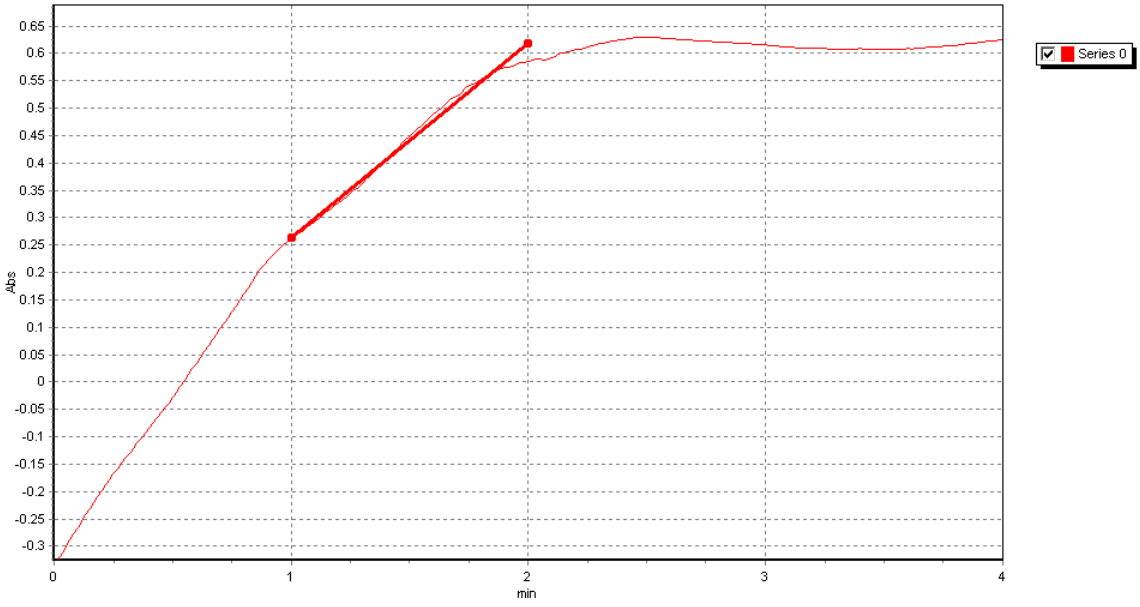
Using the above example the curve obtained would appear so:



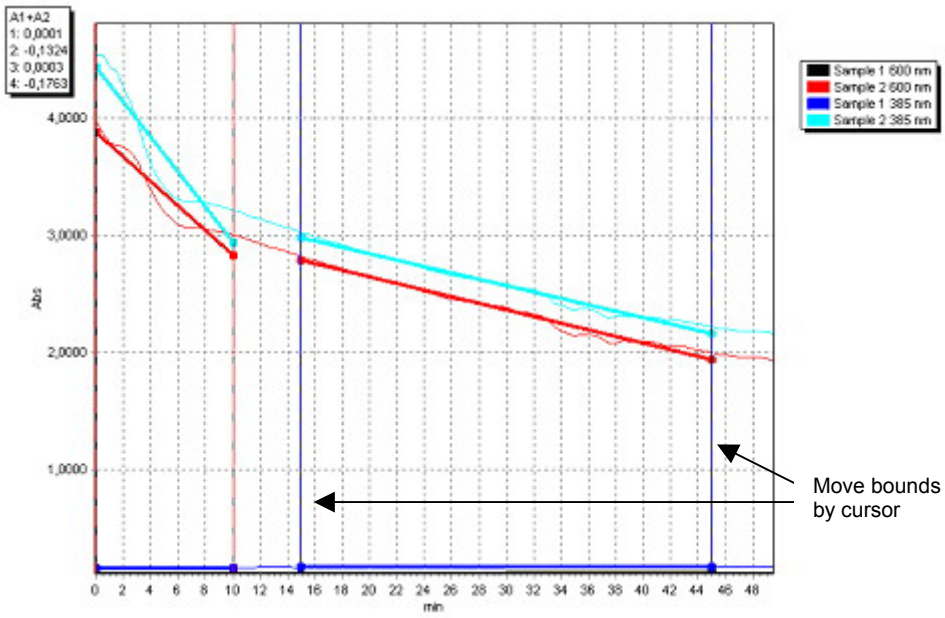
All curve calculation functions described above can also be used to modify curves used for the activity calculations.

For example it would be possible to subtract a pre-determined *Blank* value from the curve and then multiply it by a different factor, in this example the formula could be **2*(S-0.2).**

This would give the following result:



An example for defining two activities would appear so:



The bounds for activity calculation may be moved by the cursor with real-time calculation. Activities can be calculated with a mathematical function.

2.5.2.1. Activity Results

The results of the activity calculation over the requested time period can be viewed by clicking on the *Activity* tab in the *Report* screen. This displays the actual activity value for the sample plus the calculated regression line and also the correlation coefficient.

In addition the *Table* tab will show the actual activity at each point on the curve with respect to the last value. For the point n on the curve at a time t_n and an absorbance value of Abs_n the activity is calculated as

$$\mathbf{Activity = (Abs_n - Abs_{(n-1)}) / (t_n - t_{(n-1)})}$$

2.5.3. Concentration Factor

This is the most simple calculation method for concentration and is used in *Fixed Wavelength*. The concentration factor must be determined in advance if this calculation is to be used. The system uses this factor and performs the following calculation:

Concentration = Measured Absorbance value x Factor

The factor is entered as a parameter in the Acquisition screen. Click on the parameter tab to enter the screen and then enter the required value for the factor.

In this case no calibration file is required and the factor used is recorded in the report.

2.5.4. Wavelength Program functions

The *Wavelength Program* calculation functions apply only to this mode of operation and are described in the *Wavelength Program* section of this document. One more parameter appears in the calculation column.

2.5.5. Linear Calibration

The *Calibration* mode is used to create standard calibration files for the *Fixed Wavelength* mode. The *Calibration* uses a standard *Fixed Wavelength* method which must be created before running *Calibration* mode.

Method creation is possible in both the *Fixed Wavelength* and *Calibration* method screens. A method can be used to create as many calibration files as needed, the method and revision used is always linked to the calibration and is traceable.

The *Calibration* procedure is best explained using an example. In this example we will use a blank and two standards. The calibration can also be made using the cell changer.

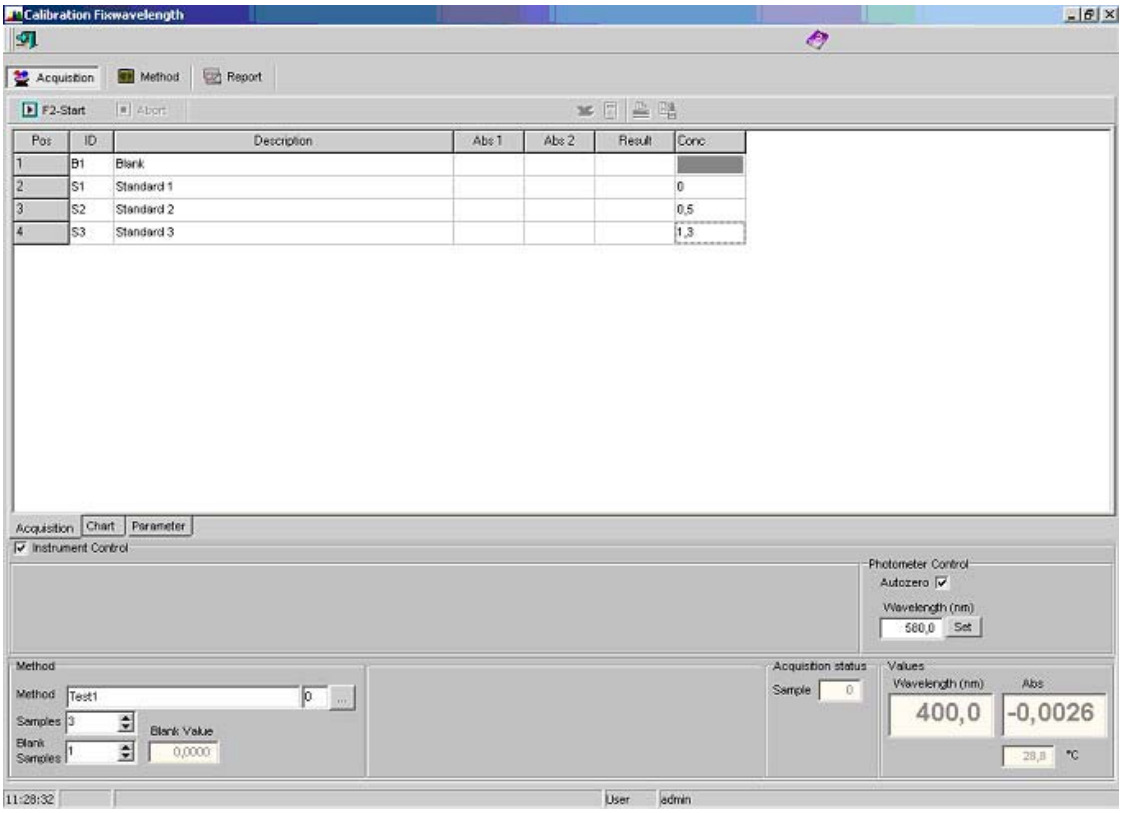
2.5.5.1. Creating a Calibration File

Select the *Calibration* mode by clicking on the *Calibration* icon in the main screen and insert the blank and the two standards in the cell changer at positions 1, 2 and 3.

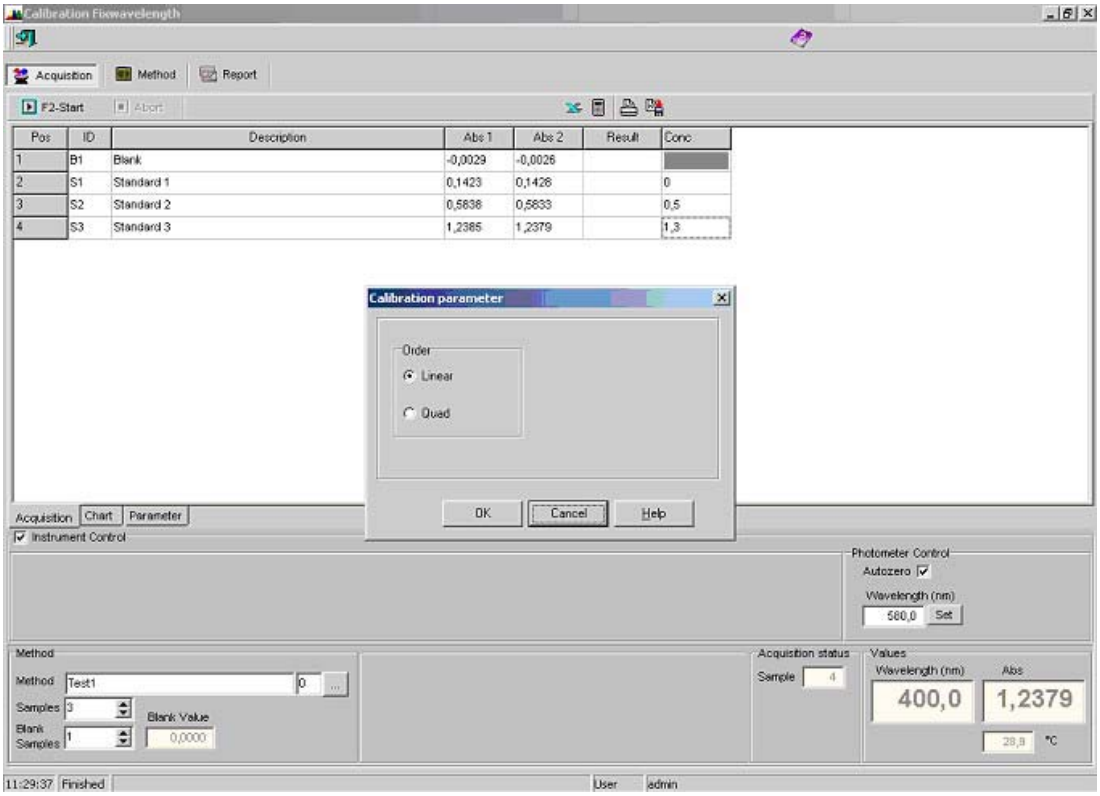
Enter the number of samples (3), the required method, a description of each sample and the concentration in the main Acquisition screen.

Clicking on the *Parameter* tab will allow entry of the units to be used for the result and also definition of an additional multiplier factor which will be used to multiply the value obtained to give the result..

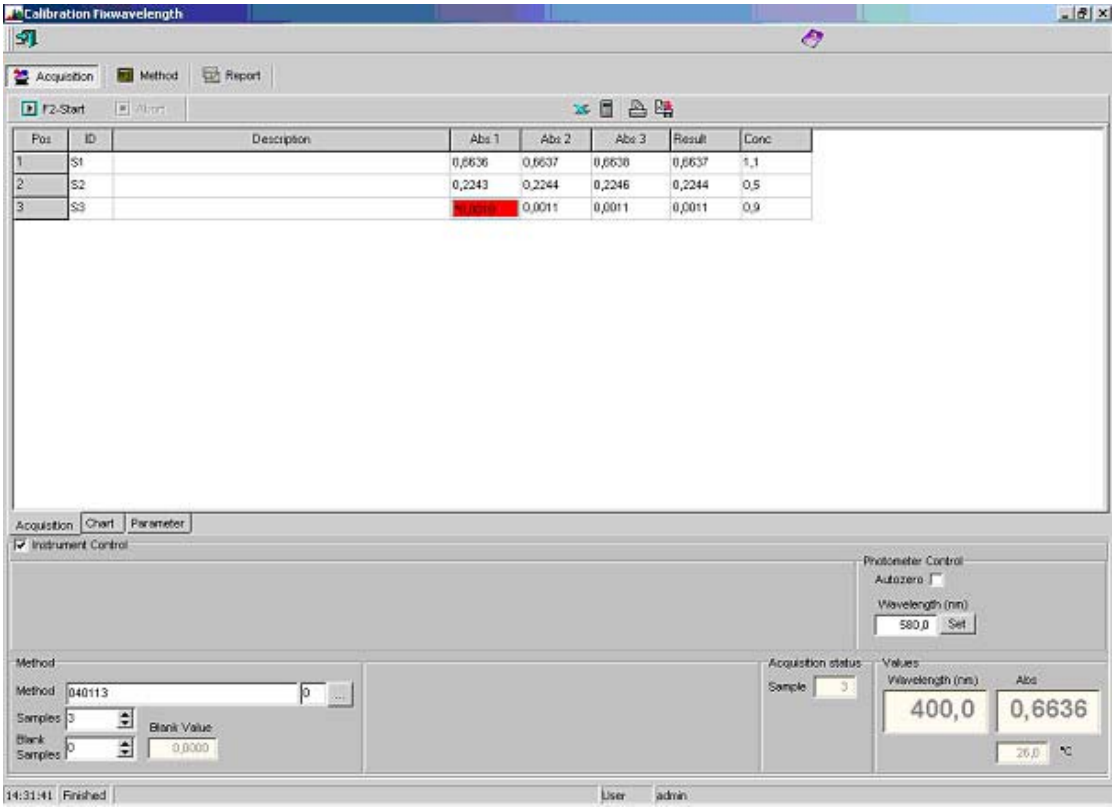
The final screen will look like this:



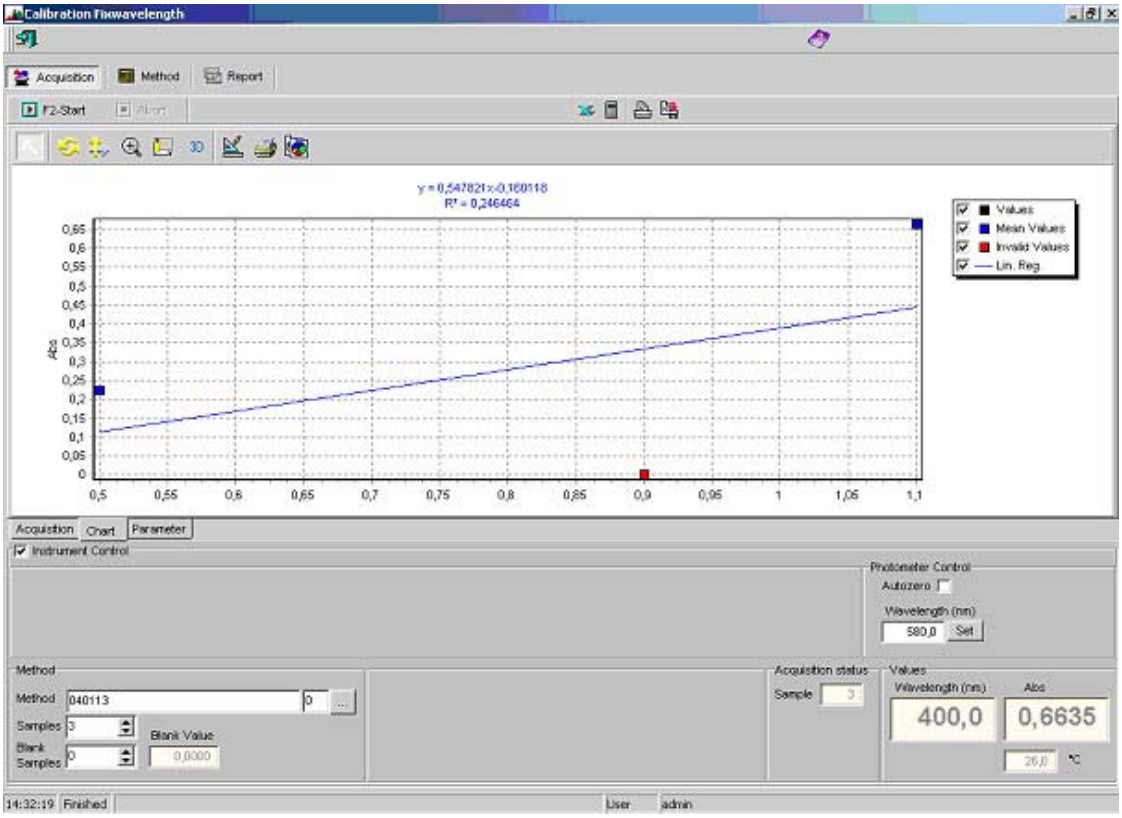
Click on *Start* to start the acquisition. Once completed the system will automatically prompt for the type of calibration required. Two possibilities are available using either a linear or quadratic regression:



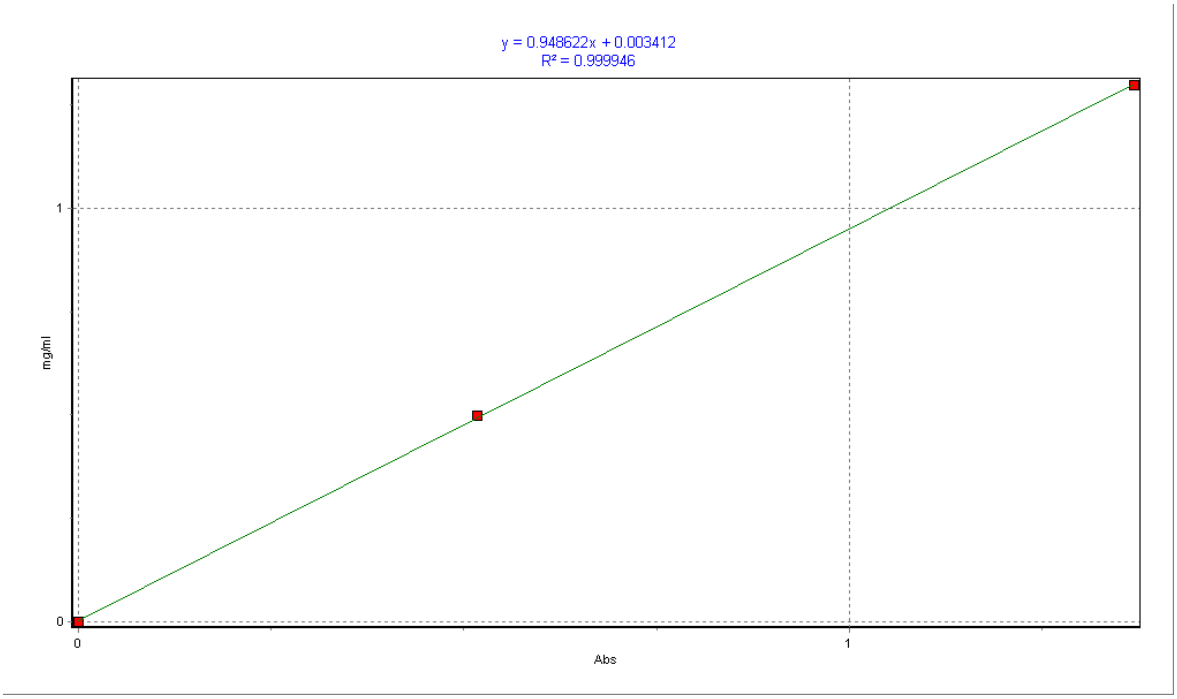
The Calibration parameter dialogue box can be recalled at any time by clicking on the calculation icon. Click the *Linear* checkbox and then save the calibration under the name required.



Values may be invalidated by double-clicking them. Invalidated values and their respective measure points in the *Chart* are marked red.



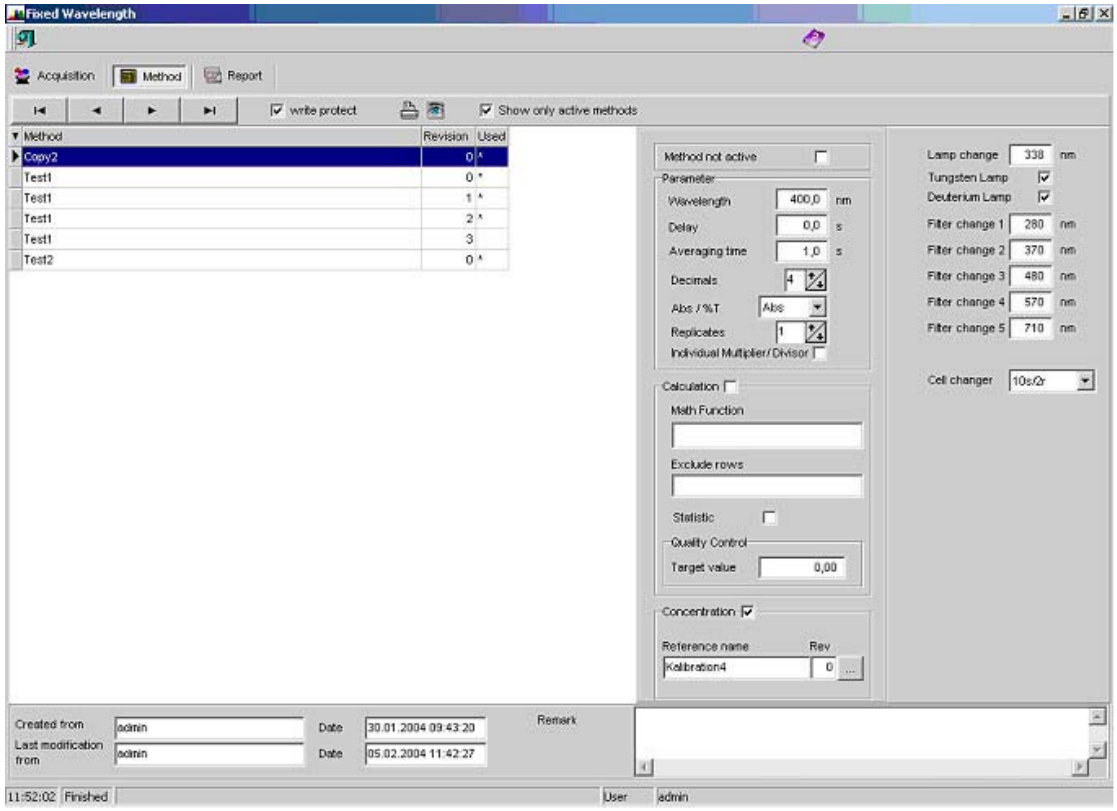
The data for a calibration can be viewed at any time by selecting the required report in the *Report* screen. Click on the Chart icon and the calibration curve will be displayed together with the regression values:



2.5.5.2. Using a Calibration Curve

The calibration curve can now be used to measure a series of unknown samples:

Exit the *Calibration* mode and select *Fixed Wavelength* and then select the *Method* screen. Here you should click the *Active* checkbox in the *Concentration* and then select the required *Calibration* as *Reference data*. Save this method and the screen should look like this:

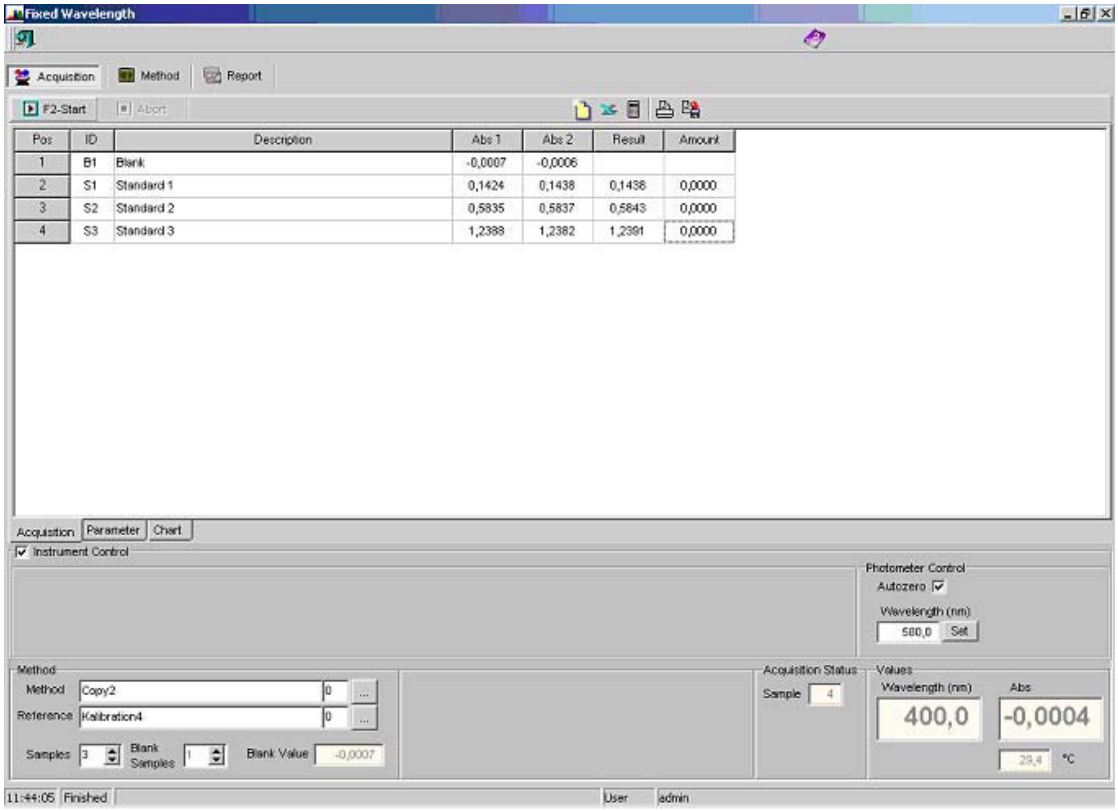


Select the *Acquisition* screen, insert the samples in the cell changer and set the number of samples to the appropriate value.

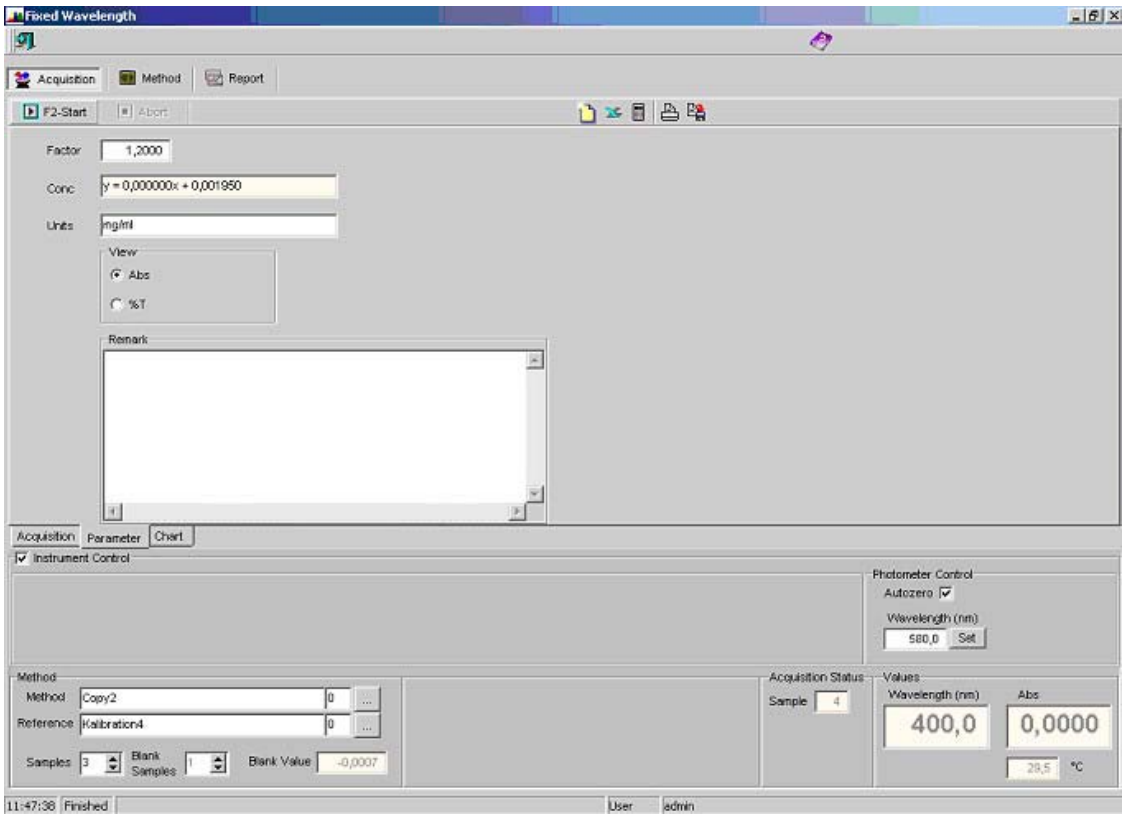
Check whether an *Autozero* is required before starting the measurement If so, click the *Autozero* checkbox in the *Acquisition* screen

Caution *Before executing the Autozero ensure that the cell changer (if used) is actually in the correct position. The Autozero will be executed at the current position which may not be position 1. Measurements with the cell changer always start from position 1.*

Press *Start*, after measurement the *Acquisition* and *Parameter* screens obtained are shown below. The main screen contains the measured absorbance values, the result and the calculated concentration values:



The *Parameter* screen contains the value used for the *Factor* used to obtain the result, the formula used to calculate the actual concentration and also the units (e.g.: µg/ml, mg/ml, etc.) may be entered:



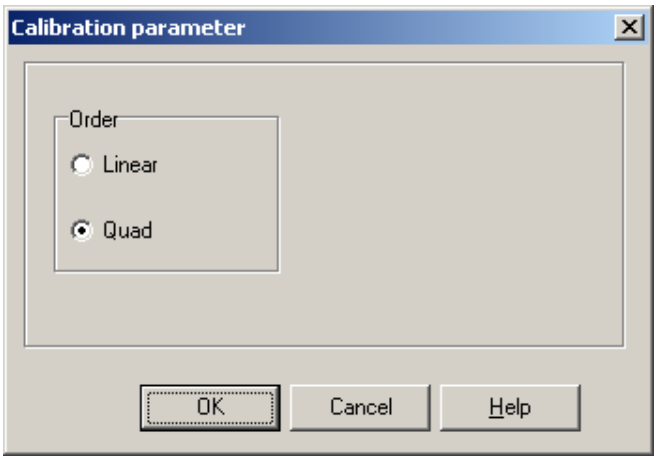
2.5.6. Quadratic Calibration

(Calculation of concentration by quadratic regression using standards)

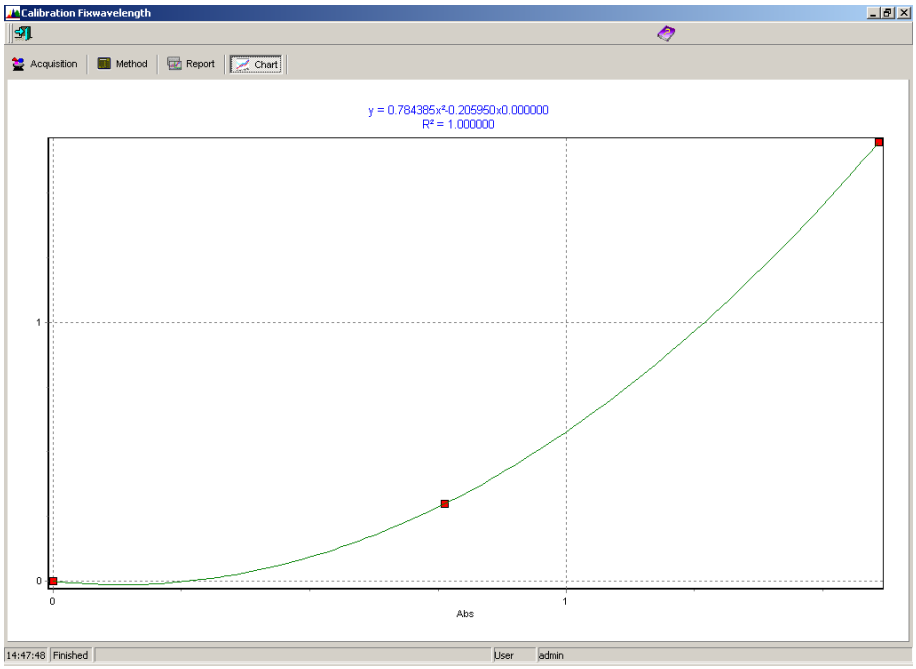
The practical use of this calculation mode is almost identical to linear interpolation (see above). One additional parameter is used with the following formula:

$$Y = Ax^2 + Bx + C$$

The process of obtaining the calibration data is identical for both the *Linear* and *Quadratic* calibration methods until selection of the calibration order is made.
Select the *Quad* function in the *Calibration* parameter dialogue:



The calibration curve will now look like this:



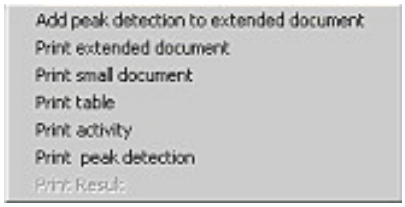
2.6. REPORTING

This section deals only with the possibilities for formatting and printing reports in the UVS software. The main focus is on the treatment of curves since all table format printouts are pre-defined.

2.6.1. Printing

The UVS software offers several possibilities for printing and formatting the various reports and data available from the system. Individual print-outs are possible for method parameters, individual results e.g. peak detection, complete reports and curve data. Each window contains its own *Printer* icon which gives a preview of the print-out.

Within the preview page the user also has the possibility to save reports under user-defined names and these reports can be viewed using the viewer of the UVS software. Click on the *Print* icon in the report screens and you will be prompted for selection of the report type required:



2.6.1.1. Add peak detection to extended document

By checking this function, the peak detection information will also be included in the extended report.

2.6.1.2. Print extended document

This will give a complete report which contains also details of the complete method used and the signature box for electronic signature confirmation.

2.6.1.3. Print small document

This is a report which contains only the basic results of a measurement and some other limited information regarding measuring conditions etc.

2.6.1.4. Print table

This report contains only the table of the measurement values and other data linked to the table.

2.6.1.5. Print activity

This report contains only the activity information and data linked to activity.

2.6.1.6. Print peak detection

This report contains only the peak detection information and data linked to peak detection.

2.6.1.7. Print result

This report contains only the result information and data linked to result.

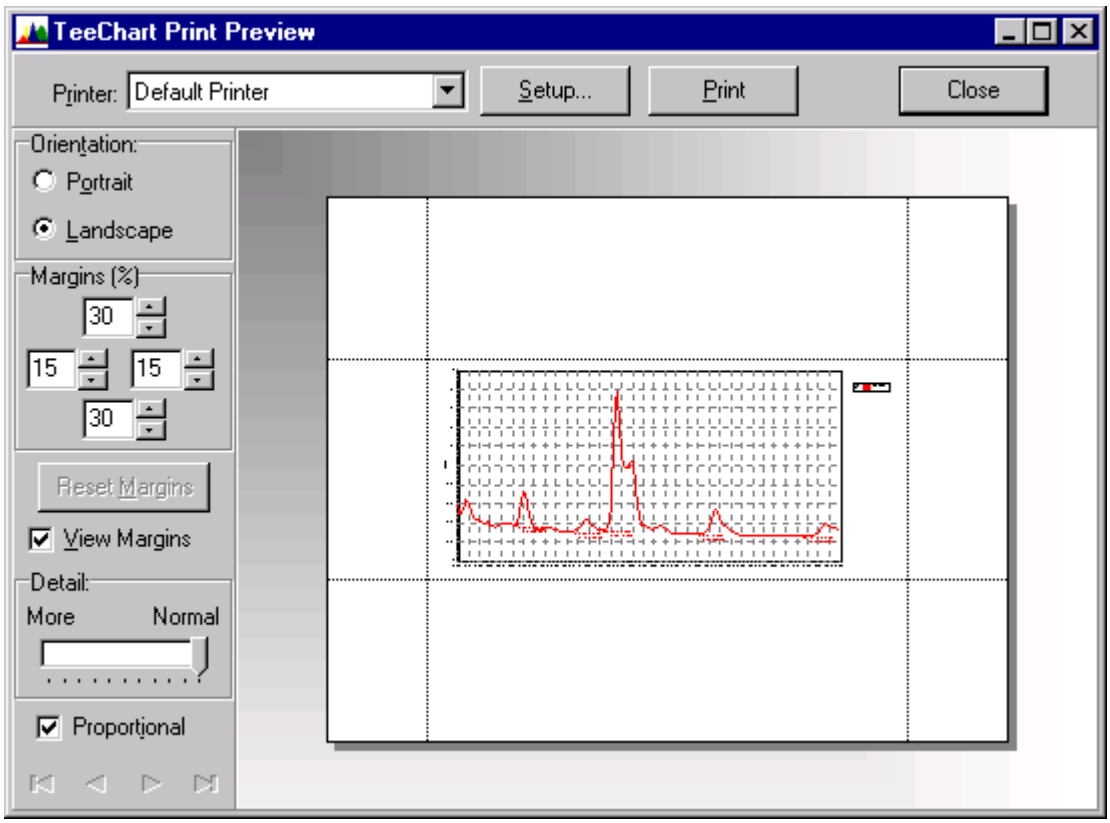
2.6.1.8. Printing

Click on either *Print small* or *Print* extended to first obtain a print preview for the requested report. Click on the *Printer* icon in the preview to print the report.

2.6.2. Direct Printing of Curves

Clicking on the *Chart* tab in the *Report* screens of modes such as *Wavelength Scan* gives the user a direct full screen display of the curves corresponding to the selected report. The appearance of the curve may be modified using the *Edit* function which is described in a separate section below.

Prints the curve as a single sheet report. Click on this icon to obtain the formatting window below. This method will only print the curve itself.



The upper bar in this dialogue box controls the actual operation and selection of the printer parameters using the standard printer installation windows.

The left-hand section of the window contains formatting functions which directly influence the print-out itself, e.g. margins, detail etc. Changes to these parameters directly influence the appearance of the print-out preview in the dialogue window. These functions are explained briefly below:

Orientation Selection of either landscape (horizontal) or portrait (vertical) format for the print-out.

Margins Spin selection boxes allow direct setting of the individual page margins.

Reset Margins Changing the preset margins automatically activates the *Reset Margins* button, click on this at any time to reset all margins to their default values. The button is not active if the margins are already set to their default values.

View Margins This checkbox allows the margin display in the preview to be switched on or off as required.

Detail Moving the scroller between normal and more increases the degree of detail shown in the curve display print-out. For example, for greater detail on the axis display move the cursor towards more until the required detail is displayed.

Proportional This returns the print-out to its original default settings without affecting the detail selected in the detail scroll bar.

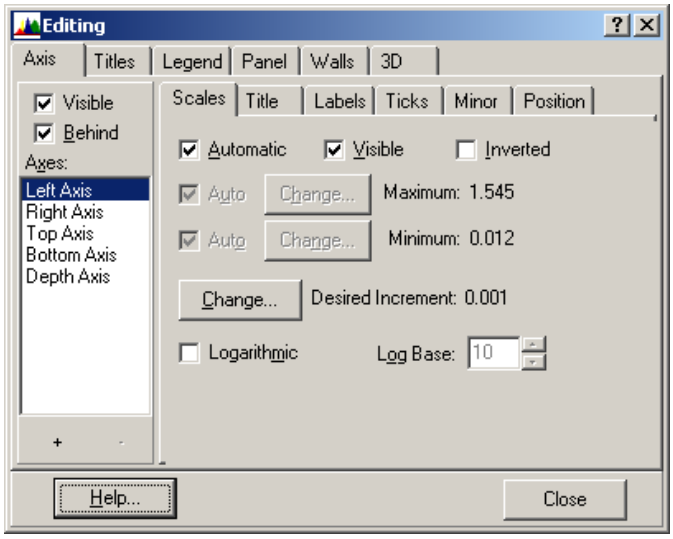
2.6.3. Editing and Formatting of Charts

The software uses a built-in editor which offers comprehensive formatting capabilities for both 2D and 3D reports. Access to this editor is obtained by clicking on the *Edit* icon. This icon is available in all screens including the *Acquisition* screen. Use of the *Edit* facility when programming a method allows immediate control of the appearance of the result without the need for time-consuming manual manipulations.

A *Help* function is provided within the *Editor* and therefore this document will only describe the more common needs with respect to formatting of charts, the user is referred to the *Help* function for additional information.

2.6.3.1. Changing the scaling (Axis)

The axis scaling is the first available tab in the *Edit* dialogue box when opened. Separate parameters can be defined for each axis and normally users would only be concerned with the so-called left and bottom axes (Y and X respectively).



The required axis to be formatted is selected by clicking in the list in the left-hand panel. Above this panel there is also a checkbox which allows the axes to be removed from the chart (visible or not). The significance of the other parameters is described briefly below:

2.6.3.1.1. Scales

Automatic The software uses dynamic scaling depending on the level of the signal obtained. In many cases this can be confusing for the user and generally it is recommended that, once known, the range should be set manually for routine operation.

Visible Check this box if you want an axis to be visible, uncheck to remove it.

Invert Checking this box will invert the chart.

Maximum If automatic is set to off, a fixed signal maximum can be defined here.

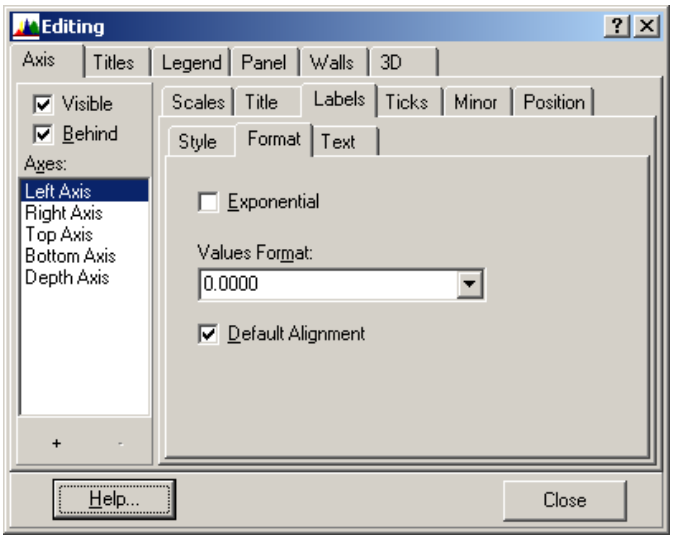
Minimum If automatic is set to off, a fixed signal minimum can be defined here.

Desired increment The desired axis increment is the minimum step between axis labels. It must be either a positive number or DateTime value. This value will be used as the initial step value. If there is not enough space for all labels, then a larger increment will be automatically calculated.
This value defines only the increment used on the scale, it is also possible to format the number of decimal places required as described below.

Logarithmic Check this box to obtain a chart based on the corresponding logarithm.

2.6.3.1.2. Decimal Format

The decimal format required can also be set from within the *Axis* tab. Click on *Labels* and then on the *Format* tab to obtain the following window:



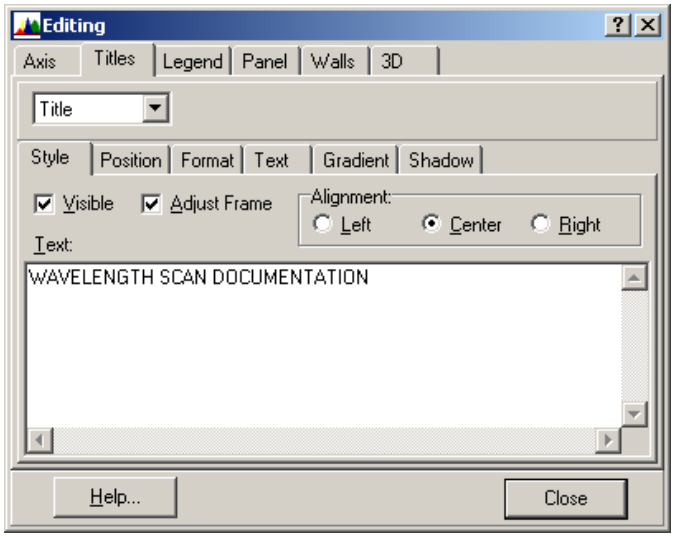
Enter the required decimal format in the “Values Format” box, e.g. for 4 decimal places enter “0.0000”.

2.6.3.1.3. Title

This allows formatting of the name to be used for a given axis, e.g. Absorbance. The tabs allow definition of the name, its alignment relative to the axis and also the font and test appearance to be used.

2.6.3.2. Titles

Normally only the definition of a chart titles in the form of either header or footer text is required. This can be done by selecting the required function using the drop-down menu and entering the text in the lower panel.

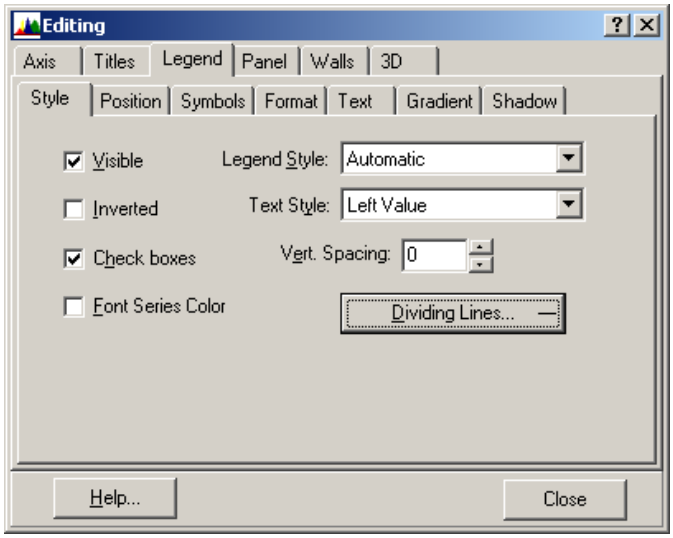


Alignment top or bottom is dependent on this selection while the horizontal position can be controlled directly from the *Alignment* box. A custom alignment using coordinates is also possible by clicking on the *Position* tab.

The remaining tabs are used to define the font type, colours, frame and certain special effects such as shadowing etc.

2.6.3.3. Legend

The legend box is used to show which curve colour corresponds to a particular sample. The default text used is “Series N” where N is the number of the sample in the batch. This default text is only used when no sample description is defined otherwise the actual description will be used automatically for the legend.



The *Style* and *Position* tabs are most likely to be used. The remaining tabs control items such as size and form of the displayed symbol and generally the applied default values will not need changing.

2.6.3.3.1. Style

Visible Unchecking this checkbox will remove the legend box from the chart.

Inverted Checking this box will cause the legend order to invert, i.e. the last sample to run will be shown at the top of the box.

Checkboxes Unchecking this box will remove the checkboxes adjacent to the text in the box. This is not recommended since the checkbox is very useful if a single curve should be removed from the overlay for any reason.

Legend Style It is recommended to maintain this setting as Automatic per default.

Text style It is recommended to maintain this setting as Left Value per default.

Vert. Spacing Controls the line spacing used within the legend box.

Dividing Lines Allows definition of the format of lines used between the individual legend entries within the box.

2.6.4. Audit Trail

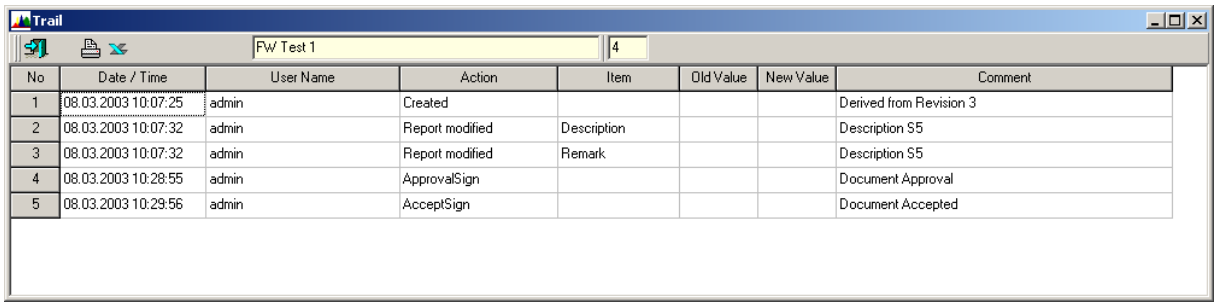
The UVS software contains an integrated *Audit Trail* which tracks all changes made to all documents after acquisition. This trail is applied to both methods and all reports and is linked to name and revision of a document.

Click on the *Audit Trail* icon in any screen to view the audit trail window for the current document and revision.

A prompt will appear asking whether you wish to view the “Report Trail”, which contains the current reports, or “Deleted Reports”, which contain audit trails for all deleted reports.

It is possible to print a report of the highlighted trail by clicking on the print icon in the top menu bar or alternatively the trail can be exported directly to Excel if required.

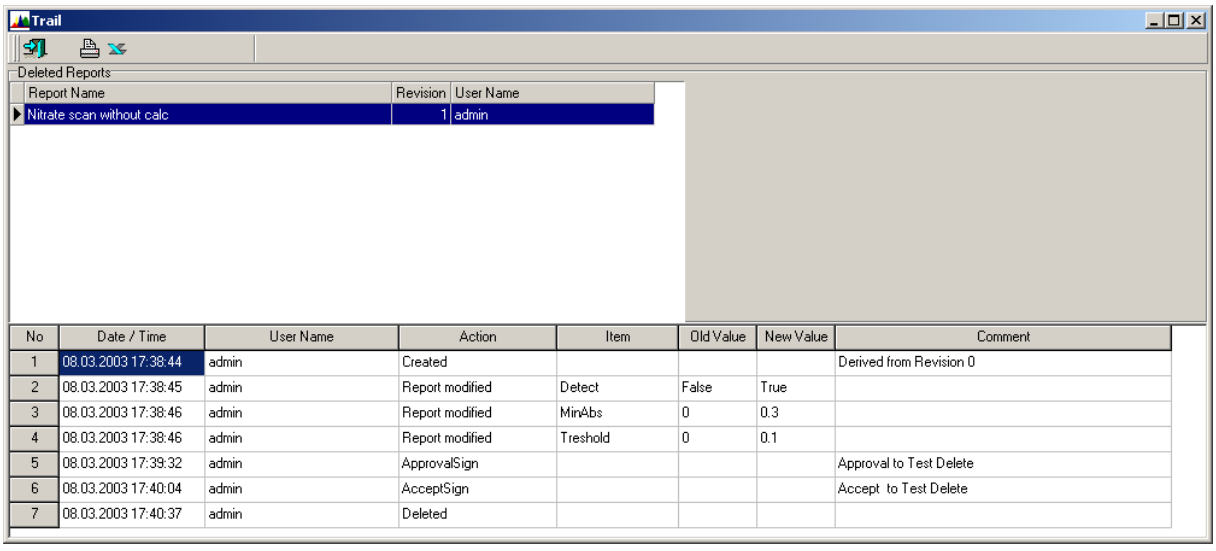
2.6.4.1. Report Trail



No	Date / Time	User Name	Action	Item	Old Value	New Value	Comment
1	08.03.2003 10:07:25	admin	Created				Derived from Revision 3
2	08.03.2003 10:07:32	admin	Report modified	Description			Description S5
3	08.03.2003 10:07:32	admin	Report modified	Remark			Description S5
4	08.03.2003 10:28:55	admin	ApprovalSign				Document Approval
5	08.03.2003 10:29:56	admin	AcceptSign				Document Accepted

2.6.4.2. Deleted Reports

The deleted report trail screen is obtained by clicking on the deleted report selection:



No	Date / Time	User Name	Action	Item	Old Value	New Value	Comment
1	08.03.2003 17:38:44	admin	Created				Derived from Revision 0
2	08.03.2003 17:38:45	admin	Report modified	Detect	False	True	
3	08.03.2003 17:38:46	admin	Report modified	MinAbs	0	0.3	
4	08.03.2003 17:38:46	admin	Report modified	Treshold	0	0.1	
5	08.03.2003 17:39:32	admin	ApprovalSign				Approval to Test Delete
6	08.03.2003 17:40:04	admin	AcceptSign				Accept to Test Delete
7	08.03.2003 17:40:37	admin	Deleted				

The upper panel contains those reports contained in the list, by clicking on one of the reports the detail for that highlighted report is shown in the lower panel.

2.6.5. Electronic Signature

The UVS software supports an electronic signature process as required under the CFR21 Part 11 Rule.

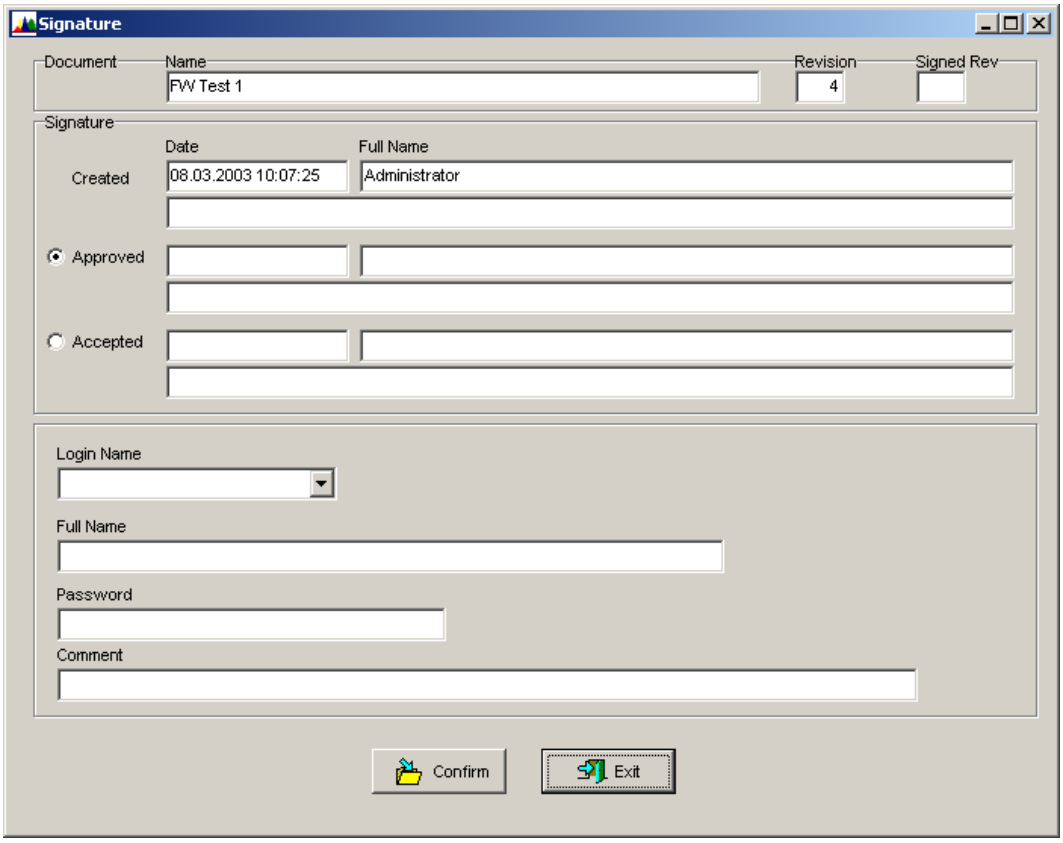
2.6.5.1. Signing a Report

In order to sign a report the signee must have been assigned the correct permission rights for the required action.

E.g. In order to be able to approve a document the user must have been assigned *Approver rights* by the administrator in the *Login* screen.

Reports can be signed even though the signees are not actually logged into the system at the time. Entry of the password is however mandatory for acceptance of any signature for *Approval* or *Acceptance* of a document.

Click on the *Signature* icon to open the following dialogue window for signing a document:



The process of signing is automated as far as is possible in order to speed up the process and support the user, a minimum number of entries need to be made. The significance of the various fields in the dialogue above are described briefly below:

Document This box contains the name of the document to be signed together with its revision number. This is entered automatically following selection of the report and the signature icon in the previous *Report* screen.

The "Signed Rev" box is used for later reference and contains the revision number of the signed report for a given document name.

Created The *Created* information is entered automatically from the audit trail for the selected report and is based on the time of last change and the currently logged in user who made the changes.

Approval The approval and acceptance areas are selectable using the check button immediately adjacent to the respective dialogues. In order to approve a document ensure that the approval button is active. All subsequent selections will be applied then to the approval process.

Acceptance The approval and acceptance areas are selectable using the check button immediately adjacent to the respective dialogues. In order to accept a document ensure that the acceptance button is active. All subsequent selections will be applied then to the acceptance process.

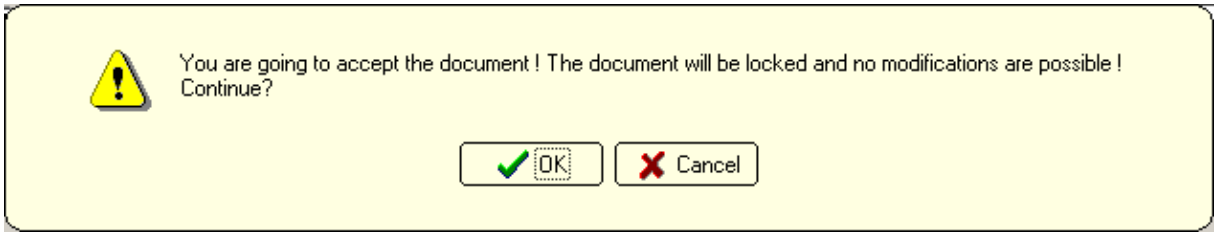
Login Name This is a drop-down selection list which allows selection of the user who is executing the signature. Only those users with the appropriate rights are displayed in the list, i.e. for acceptance only users with acceptance rights will be displayed. Select your user name from the list.

Full Name The full name is entered automatically once the user name has been selected as described above. The full name is defined initially as part of the login definitions and cannot be changed here.

Password Entry of the user password is mandatory before any signature process can be successfully concluded.

Comment Here a comment relating to the signature can be entered and this will be stored with the other signature details and also shown on all printed reports.

Once a document has been signed off and accepted it is no longer possible to change that document, therefore there are a series of prompts appearing to ensure that the user is aware of this process before actually proceeding. The final prompt appears after the signee has confirmed that the document should be signed off and is the final safety check before closing the document:



Caution *Only click on OK here if you are absolutely certain that the document in its current form is acceptable.*

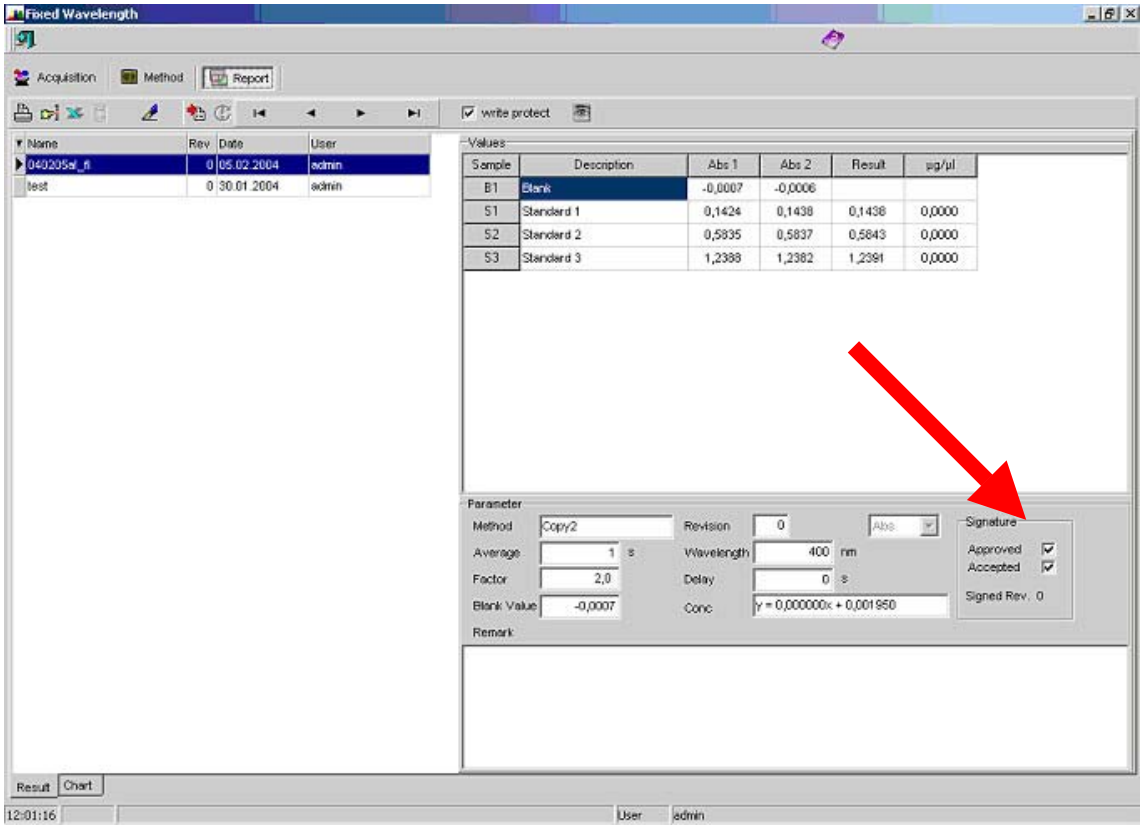
2.6.5.2. Signature Status Indications

2.6.5.2.1. Quick Overview

There are various indications to show the status of a report and whether it has in fact been signed off and accepted.

All signed reports in the list are shown with a shaded background so that the user can immediately identify those reports in the list which have been signed and accepted.

The status of a signed report in the report list is shown automatically when the report is selected in the report list:

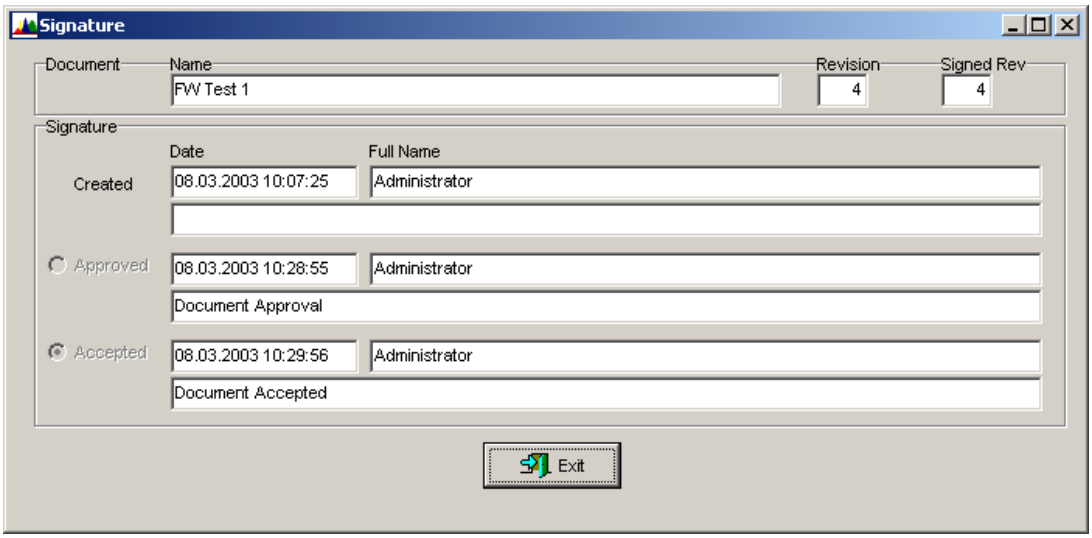


The *Approval* and *Accepted* checkboxes are only checked for a signed report. The *Signed Rev* field always carries the revision number of the signed report, if there is no entry in this field then no signed report exists for that particular named report.

It is also possible to partially sign a report, e.g. only approval, and in this case only the *Approval* box would be checked.

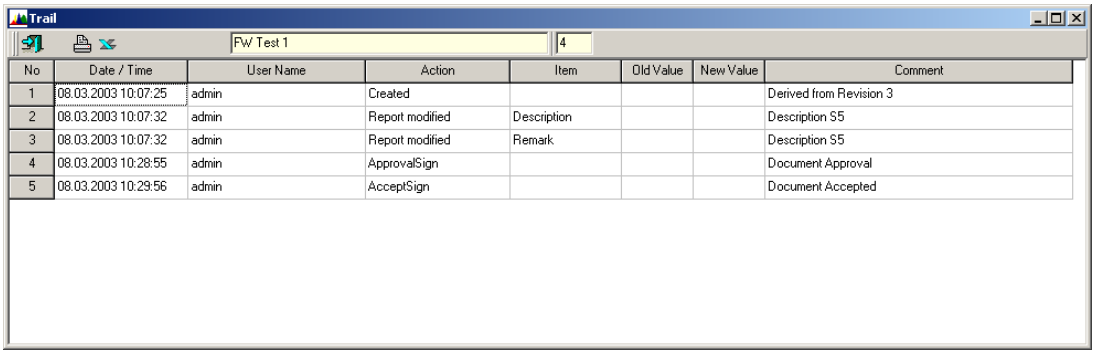
2.6.5.2.2. Detail Overview

By clicking on the *Signature* icon it is possible to see the complete details of the signature entries for the given report. Select the report from the list and click on the icon to obtain the *Signature* information:



2.6.5.2.3. Signature Audit Trail

The signature details are also recorded as part of the audit trail process and can be viewed in the report trail:



2.6.5.3. Deleting a Signed Report

For a given report it is only possible to have one signed report with the respective report name. In rare cases it may be necessary to correct a signed report after signature and then re-sign it.

The UVS software allows a signed report to be deleted by users with administrator rights only and the deletion is recorded in a separate *Deleted Reports Audit Trail*.

A new report can be signed in the normal way as described above.

3. OPTIONS AND ACCESSORIES

3.1. AUTOMATIC CELL CHANGER

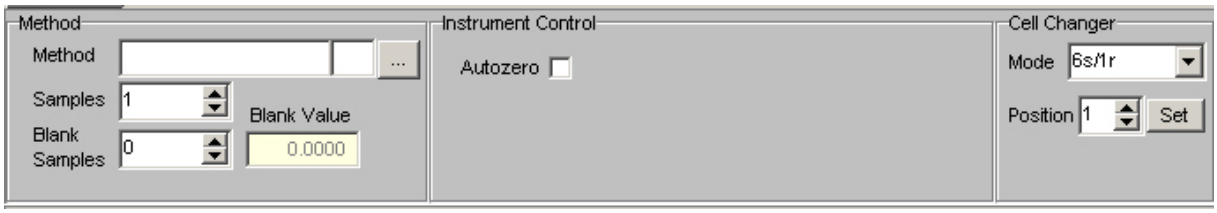
3.1.1. Installation

Switch off the instrument and plug in the cable on the accessory board connector in the sample compartment. Switch on the instrument and start the UVS software. The cell changer will be recognised by the software during the initialisation process.

Access to the cell changer is possible in all modes using either direct control in the acquisition screen for single measurements or integration into a method for automatic processing of samples. The cell changer mode can be set as described below during either of these processes..

3.1.2. Cell Changer Mode (only UVSX)

The cell changer allows three different operation modes and the mode is selectable via the *Cell Changer* dialogue in, for example, the *Acquisition* screen:

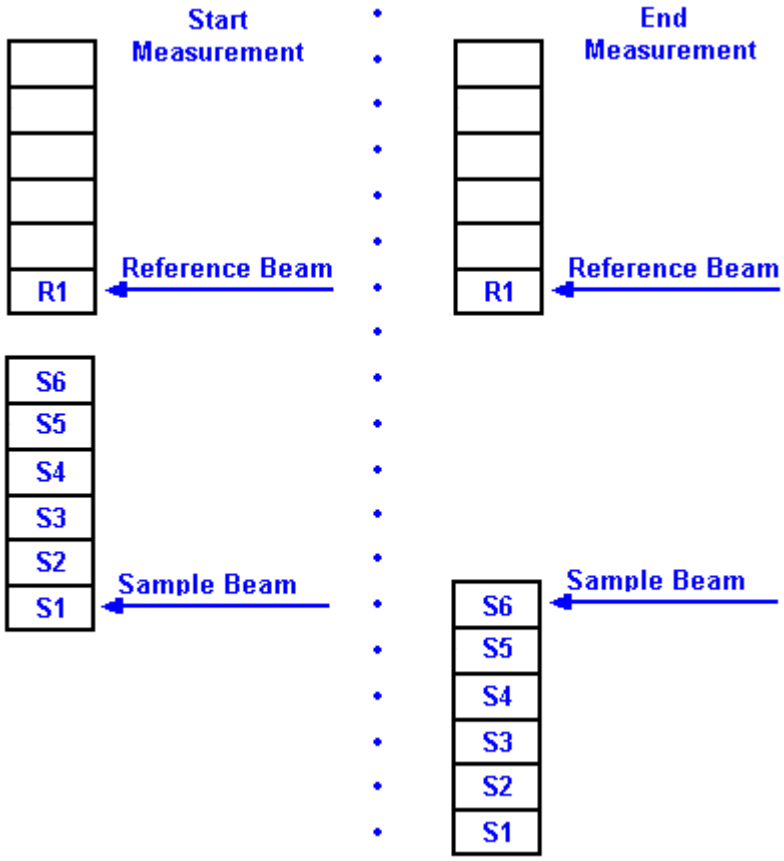


Click on the drop-down menu in *Mode* to select the required mode from a list.

3.1.2.1. 6 samples / 1 reference.

This mode allows measurement of 6 samples in the sample cell holder against 1 reference in position 1 of the reference cell holder. Only the sample cell holder moves during measurement.

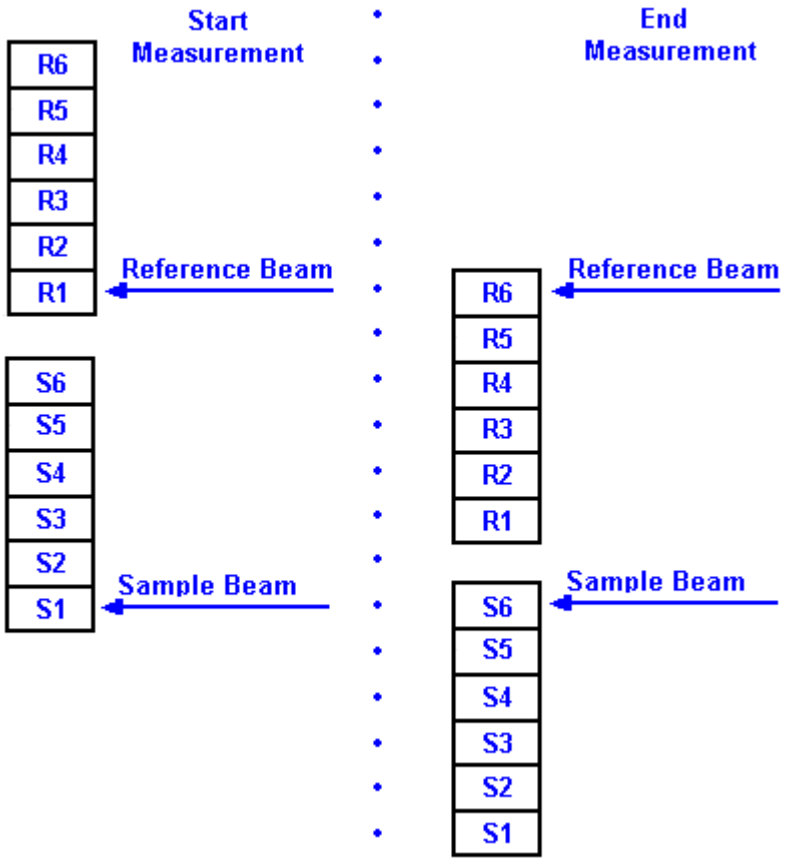
The figure below shows the cell holder positions at start and end of a measurement if all 6 cells are measured.



3.1.2.2. 6 samples / 6 references.

This mode allows measurement of 6 samples in the sample cell holder against 6 references in the reference cell holder. Both holders move simultaneously during measurement.

The figure below shows the cell holder positions at start and end of a measurement if all 6 cells are measured.

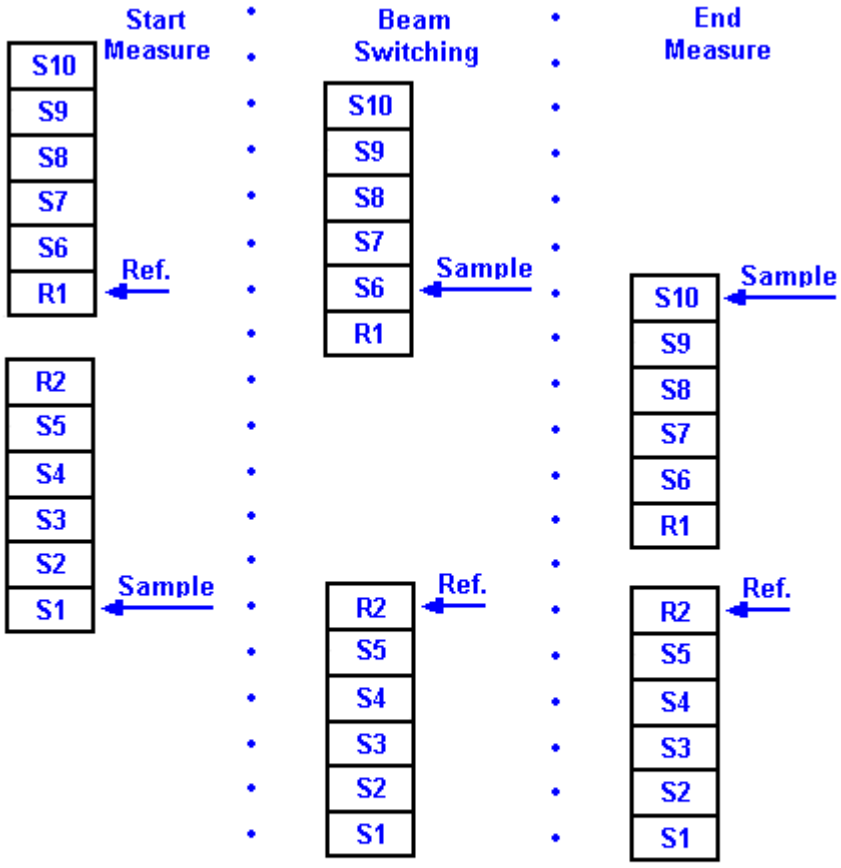


3.1.2.3. 10 samples / 2 references.

This mode allows measurement of 10 samples (5 in the sample cell holder and 5 in the reference cell holder) against 2 references:

- Ref. 1 in position 1 of the ref. cell holder
- Ref. 2 in position 6 of the sample cell holder

Both holders move independently during measurement:

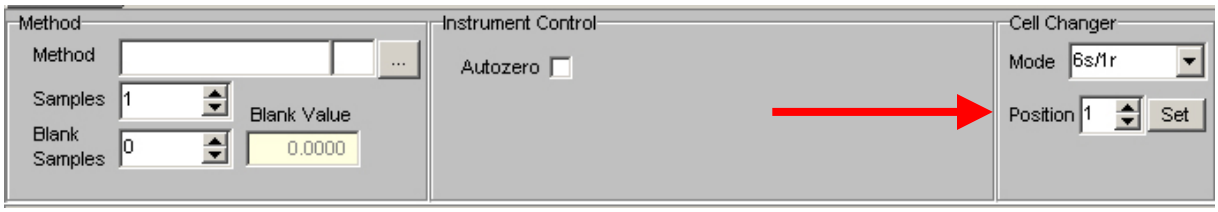


If more than 5 samples are selected in the 10 samples against 2 references mode the sample and reference beams are exchanged after the fifth sample has been measured. This unique 'beam switching' is possible due to the fact that both beams have a fully symmetric optical layout combined with symmetrical data acquisition electronics.

3.1.2.4. Manual operation (only UVSX)

The cell changer can be moved manually using the *Position* spinbox in the *Acquisition* screen. The sample position will be set automatically depending on the mode setting (see above).

Select the required sample position and the press the *Set* button, the cell changer will then move to the required position for measurement.



3.1.3. Cell Changer operation in the different system methods

3.1.3.1. Auto rate assay

In this method the instrument can measure up to ten samples simultaneously when the cell changer is in use. Measurement starts with the first reading on sample 1. The cell changer then moves to the next position and measures the first reading on sample 2. This process continues until all selected samples (parameter No. OF SAMPLES) have been measured once. The instrument will then continue measurement with the second reading on sample 1 and all other samples. The whole process is repeated until the selected number of readings has been measured. Up to ten curves (depending on the selected number of samples) can be displayed on the screen during measurement.

3.1.3.2. Fixed Wavelength

Measurement starts with the first sample. After the selected *Averaging Time* the cell changer will move to the second sample. Only one reading per sample is measured and displayed. The cell changer can also be used to measure standards in *Calibration* mode.

3.1.3.3. Wavelength Scan

The complete scan is carried out on the first sample before the cell changer moves to the second position and measurement of sample 2 is carried out. This process continues until the selected No. of samples has been measured.

3.1.3.4. Time Drive

The complete Time Drive is carried out on the first sample before the cell changer moves to the second position and measurement of sample 2 is carried out. This process continues until the selected No. of samples has been measured.

3.1.3.5. Wavelength Program

All samples are measured at the first wavelength, then the wavelength is changed to the second one and all samples are measured again. This process will be repeated until all wavelengths for all samples have been measured.

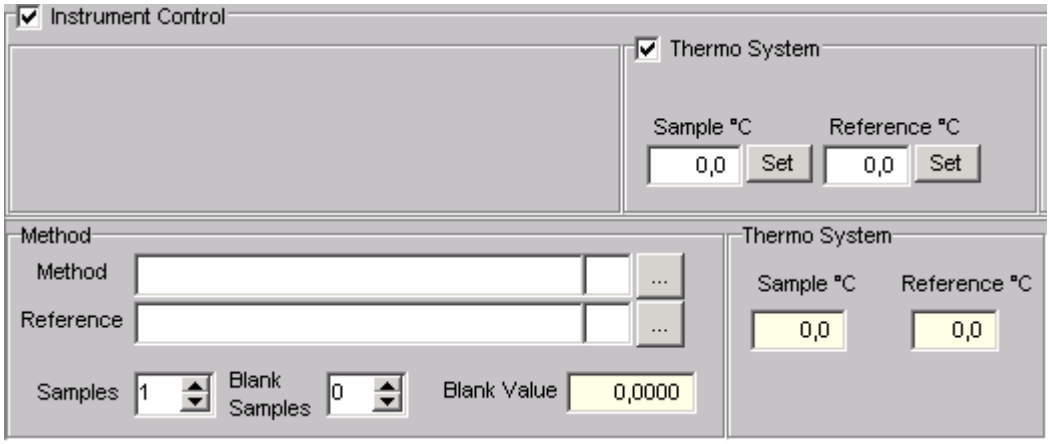
3.2. Thermosystem / Thermopack

3.2.1. Installation

Connect the thermosystem or thermopack the serial line COM 1. Start the UVS Software, the thermosystem / thermopack will be detected.

3.2.1.1. Manual operation

If the thermosystem / thermopack is detected an additional window is shown in the control/display area of the acquisition window.



Enter the required sample or reference value and the press the *Set* button, the thermosystem / thermopack will then move to the required temperature value.

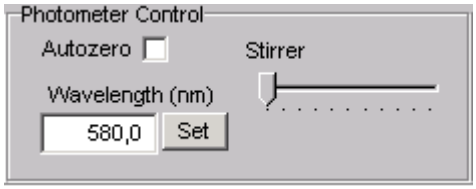
If a thermopack is detected only the sample is shown.

3.3. Stirrer (only UVSX)

3.3.1. Installation

Switch off the instrument and plug in the cable on the accessory board connector in the sample compartment. Switch on the instrument and start the UVS software. The stirrer will be recognised by the software during the initialisation process.

Access to the stirrer is possible in all modes using either direct control in the acquisition screen.



Move the track bar to set the stirrer speed, the stirrer will follow immediately.